A Joint Experimental/Computational Study of Non-idealities in Practical Rotating Detonation Engines

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2016 UTSR Workshop, November 1-3, 2016

Blacksburg, VA

DOE FE0025315 with Dr. Mark C. Freeman as Program Monitor

Outline

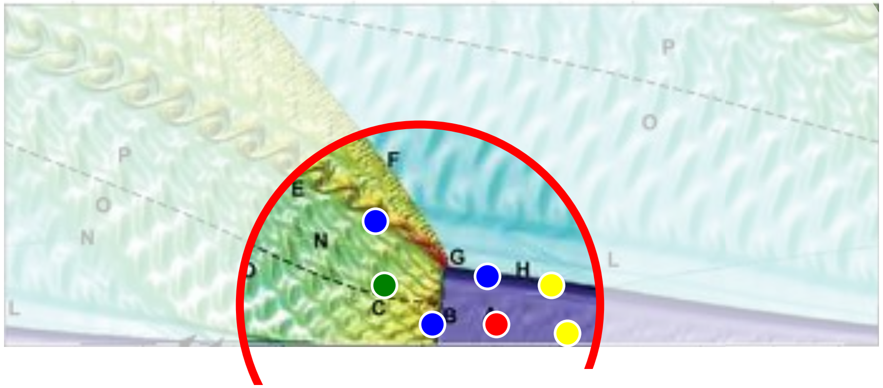
- Introduction to the problem and general approach
- Experimental activities
- Computational activities

Overarching objectives

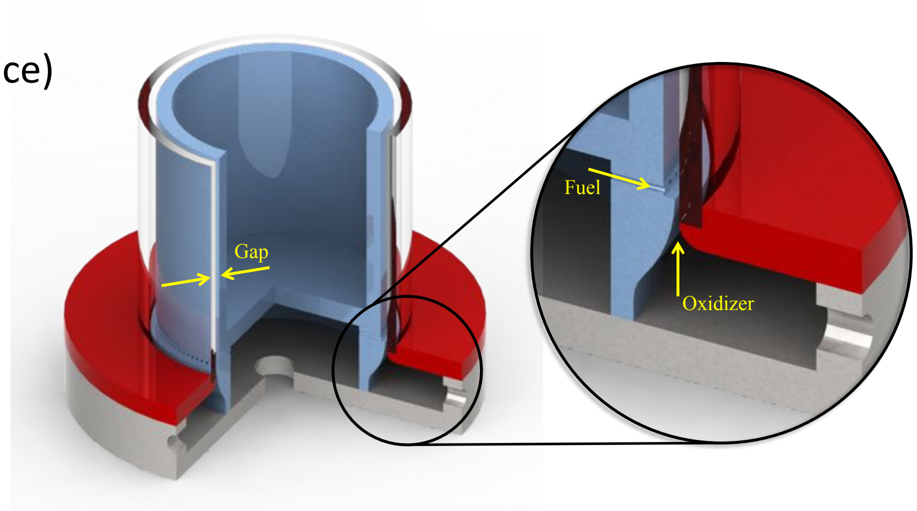
- **Use laser diagnostics to:**
  - Develop canonical systems for RDE investigation
  - Understand the physics of RDE in lab- and full-scale configurations
  - Provide data for validation

- **Use high-fidelity simulations to:**
  - Understand basic detonation physics
  - Simulate full scale RDEs

Overarching goal:
investigate non-idealities and their link to loss of pressure gain



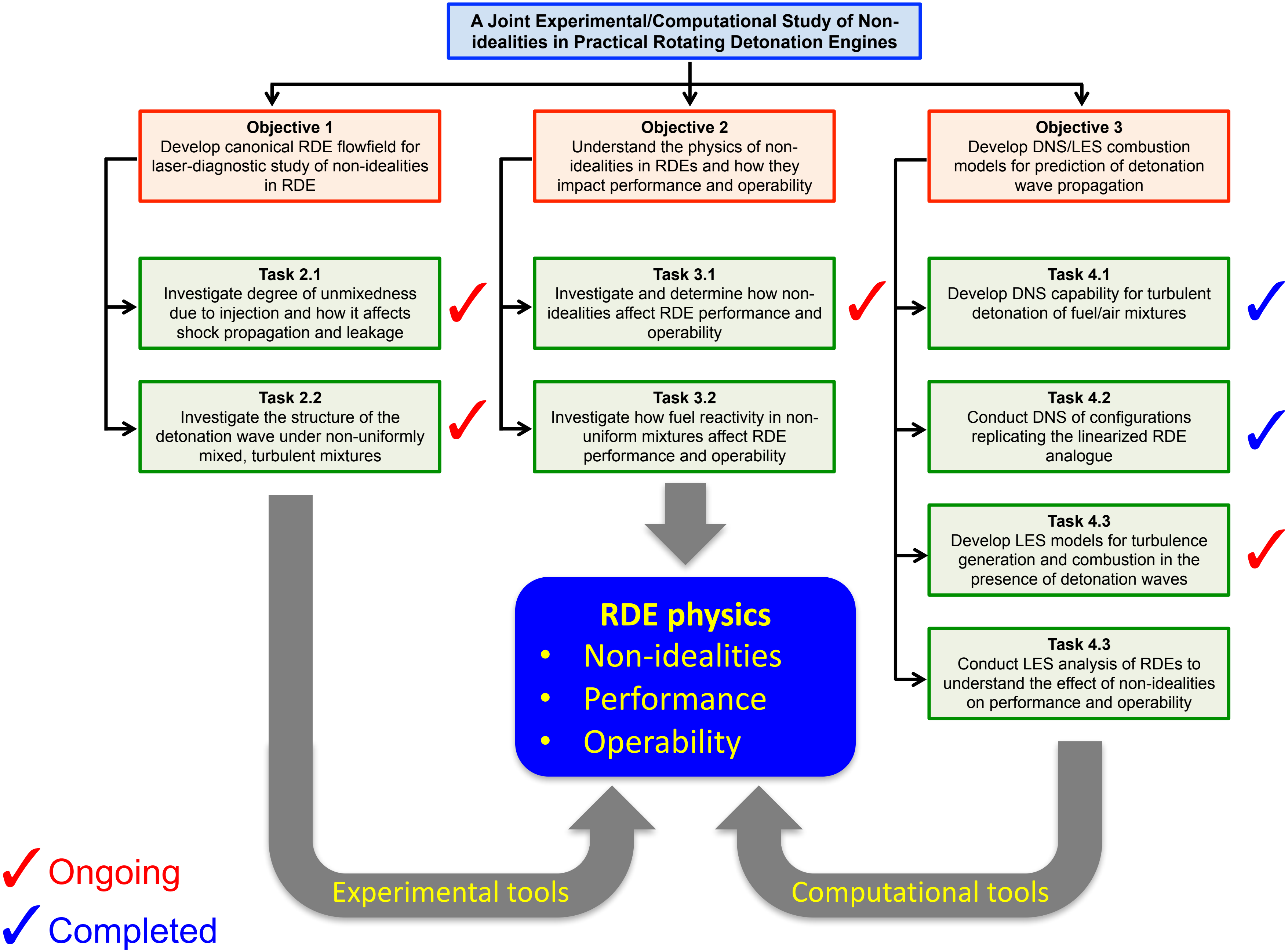
- Detonation non-idealities
  - Incomplete fuel/air mixing
  - Fuel/air charge stratification
  - Mixture leakage (incomplete heat release)
  - Parasitic combustion:
    - Premature ignition (e.g., burnt/unburnt interface)
    - Stabilization of deflagration (flame)
  - Detonation-induced flow instabilities
    - Richtmyer-Meshkov (R-M) instability
    - Kelvin-Helmholtz (K-H) instability



- They lead to loss in pressure gain
  - Linked to loss of detonation propagation
- Additional losses exist during flow expansion
  - Secondary shock and (multiple) oblique shock
  - Flow instabilities (e.g., K-H instability)
  - Mixture leakage through burn/unburnt interface

From:
(top) Nordeen et al., AIAA 2011-0803

Objectives and tasks



Our approach: a multi-level physics study

Practical RDE

↓

Unit-physics decomposition

↓

Diagnostics

- Laser-based imaging
- Mixing measurement
- Detonation structure
- Temperature and species imaging

Injection & mixing

- Multiple injection mixing
- Shock-induced mixing
- DNS/LES modeling
- Experiments

Turbulence & detonations

- Linear analogue
- Detonations in stratified mixtures
- DNS/LES modeling
- Experiments

Detailed modeling

- Variable mixture ignition model
- Homogeneous reactor model with tabulated ignition times
- Non-equilibrium

Today we will discuss

- **Experimental component:**
  - Initial investigation of shock-induced mixing
  - Development of lab- and full-scale RDE systems

- **Computational component:**
  - Effect of nonequilibrium on detonation cell size
  - Effect of injector mixing on detonation propagation

Outline

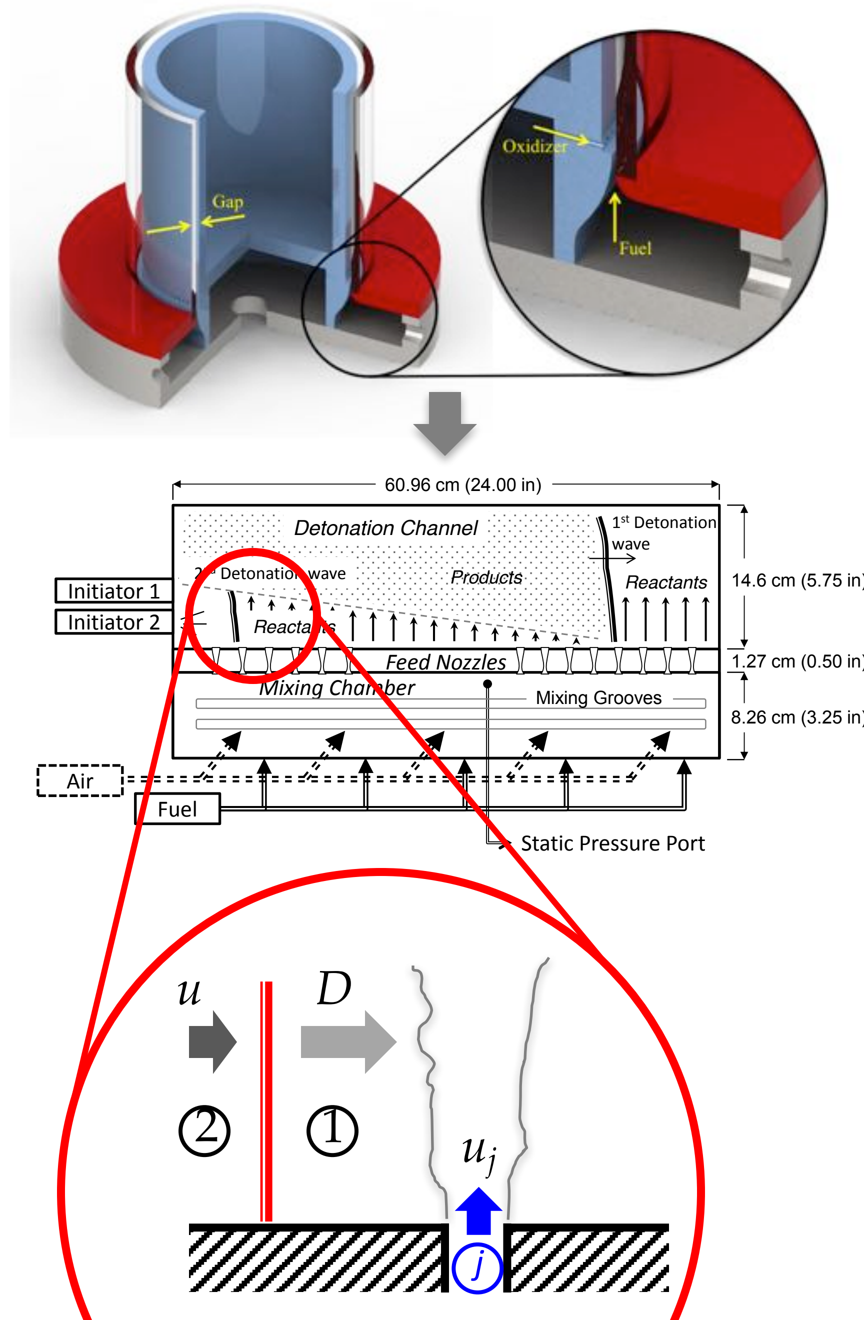
- Introduction to the problem and general approach
- Experimental activities
- Computational activities

Planned experimental multi-level approach

RDE full system:
- Link between mixing and performance
- Design from ISSI/AFRL

Linearized analogue:
- Detonation structure
- Detonation/turbulence interaction
- Detonation in stratified mixtures
- Design from ISSI/AFRL

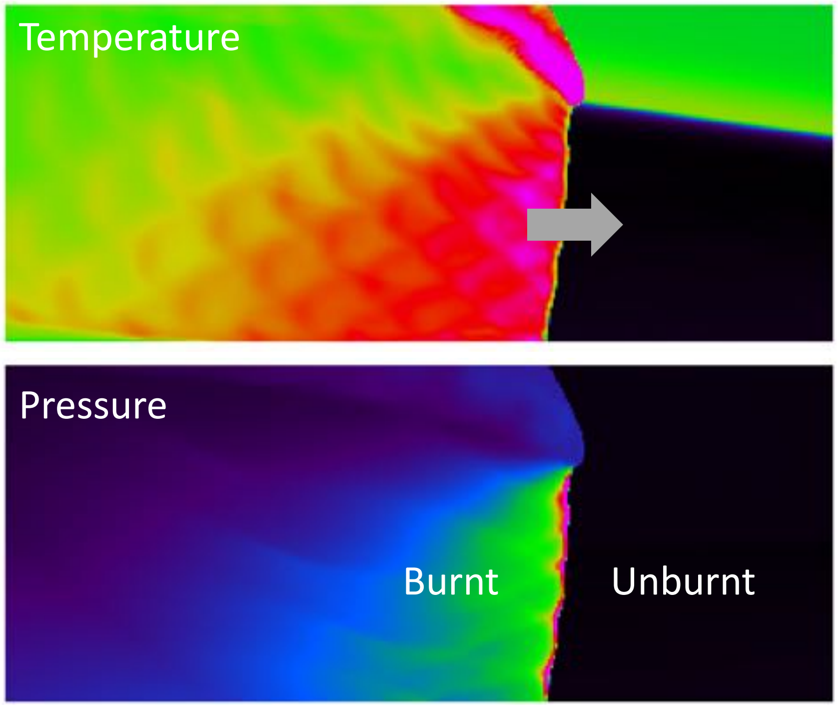
Single or multiple injectors:
- Mixing studies
- Shock-induced mixing
- Our starting point



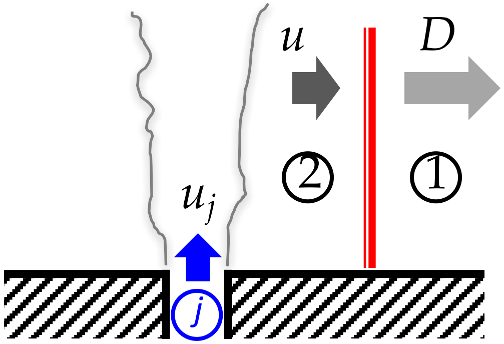
Hierarchy

Shock-induced mixing: detonation/shock analogy

Detonation



Shock analogy



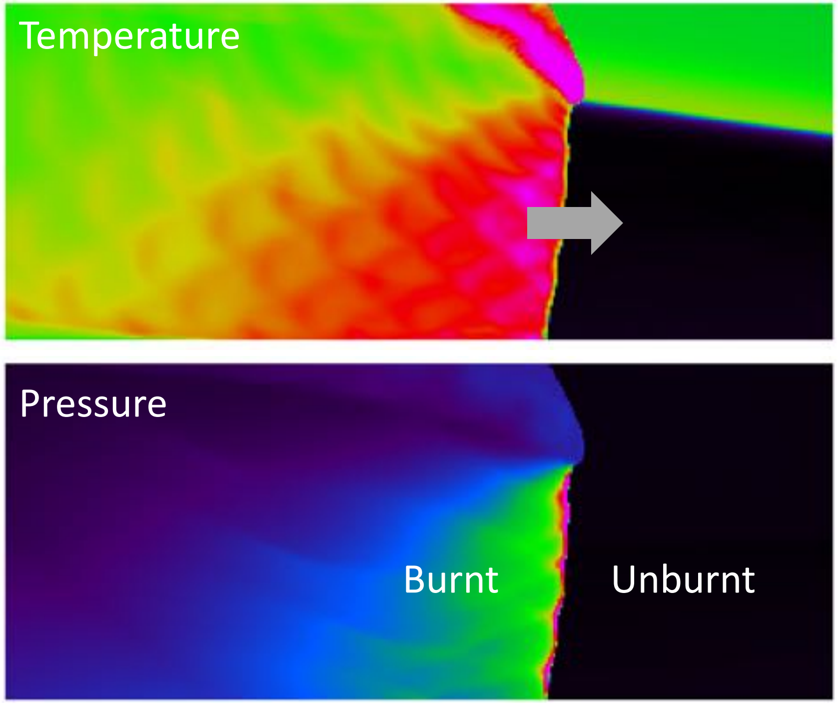
$$\frac{u_2}{u_j} \ \& \ \frac{\rho_2}{\rho_j}$$

- Important parameters
  - Wave speed *D* (Mach number)
  - Jet-to-ambient (induced flow) density and velocity ratios
  - Injection pressure and configuration

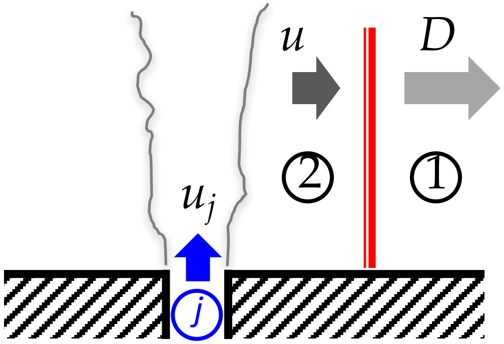
From: Schwer D. A. and Kailasanath K., AIAA 2010-6880

Shock-induced mixing: detonation/shock analogy

Detonation



Shock analogy



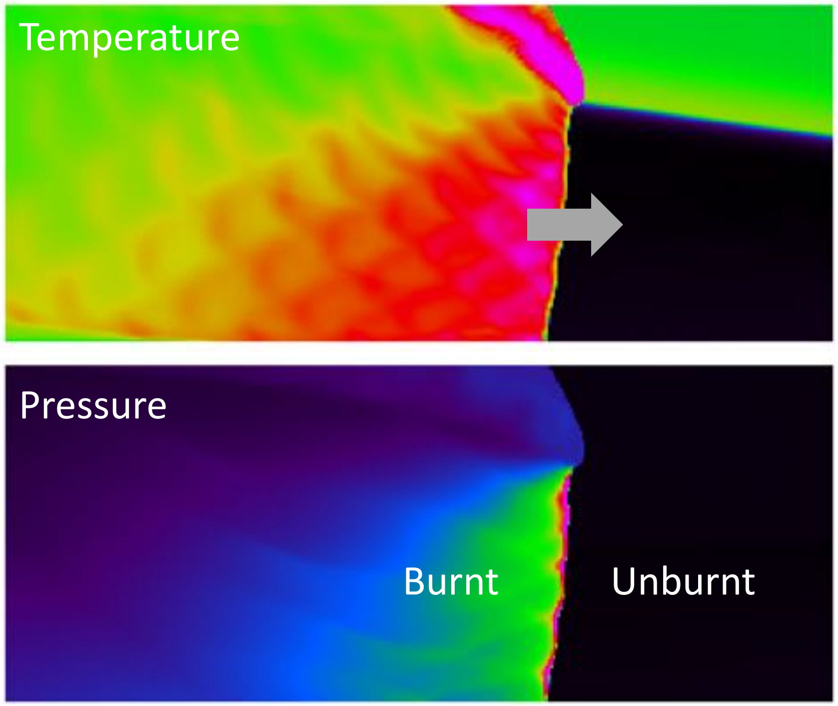
$$\frac{u_2}{u_j} \; \& \; \frac{\rho_2}{\rho_j}$$

- Open questions:
  - Does the analogy hold?
    - In what ways mixing in a non-detonating flow captures mixing in detonation
  - Impact of shock compression on turbulent mixing and structure

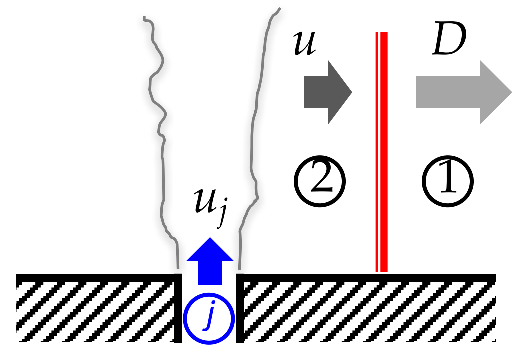
From: Schwer D. A. and Kailasanath K., AIAA 2010-6880

Shock-induced mixing: detonation/shock analogy

Detonation



Shock analogy

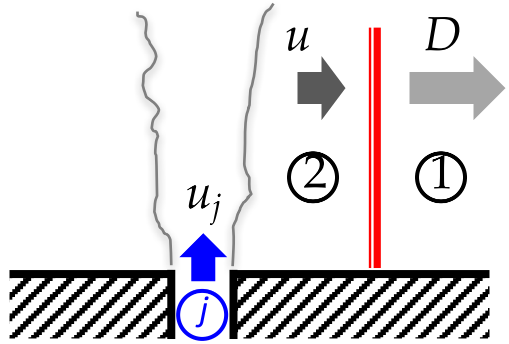


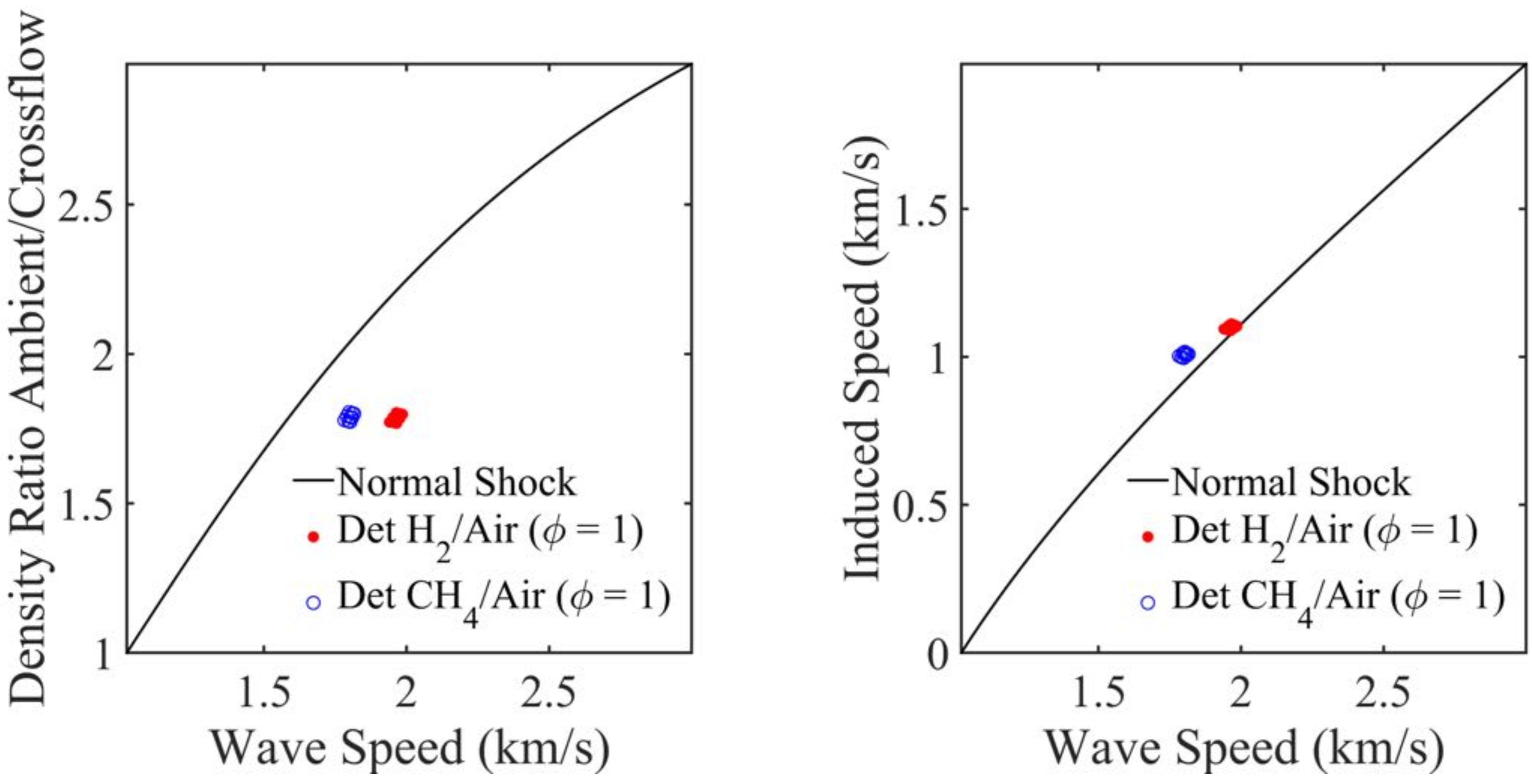
$$\frac{u_2}{u_j} \;\&\; \frac{\rho_2}{\rho_j}$$

- We answer the questions by combining:
  - Experimentation in canonical flow
  - High-fidelity simulations of detonating and non-detonating flowfield (multiple-injectors)

From: Schwer D. A. and Kailasanath K., AIAA 2010-6880

Scaling of detonation/shock analogy





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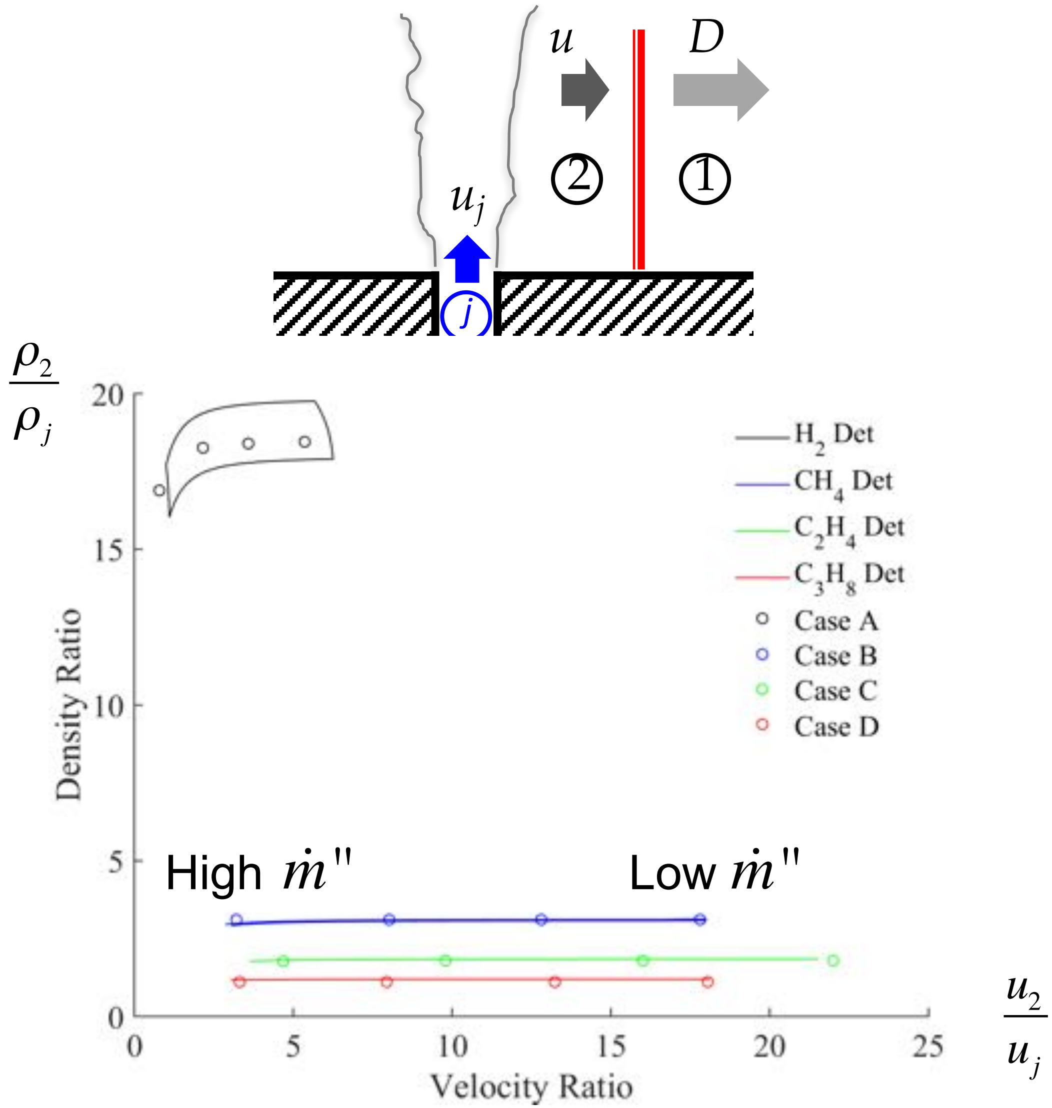
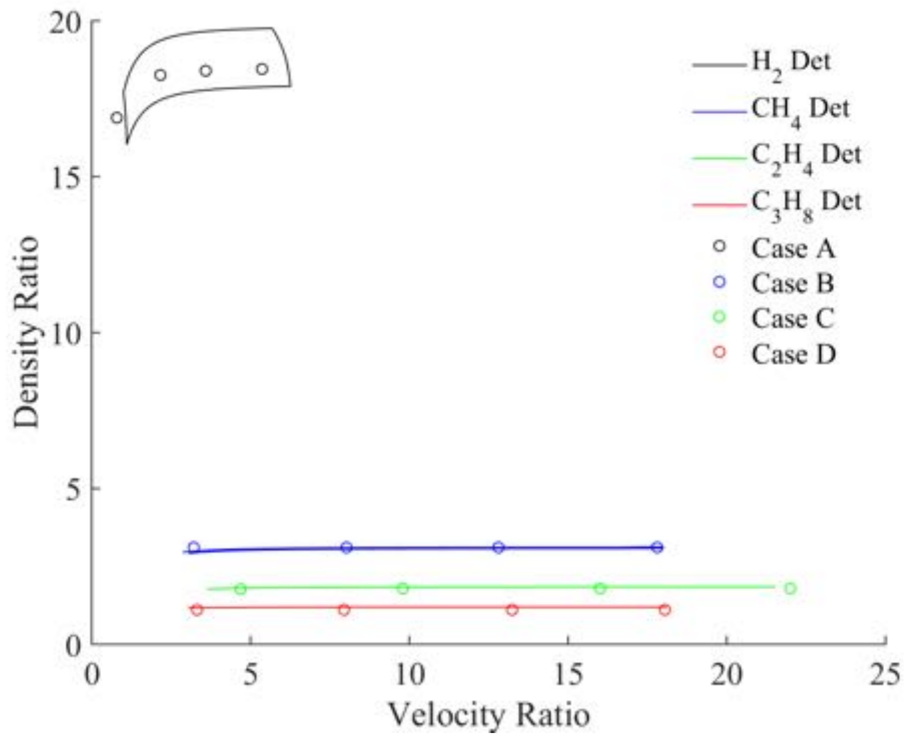


$\dot{m}''$: Mass flux

Scaling of detonation/shock analogy

Case	Ambient	Jet	Wave Mach	Detonation
A	Air	Helium	1.9	H_2/Air
B	Air	Methane	1.4	CH_4/Air
C	Air	DME	2.1	C_2H_2/Air
D	Air	DME	1.5	C_3H_8/Air



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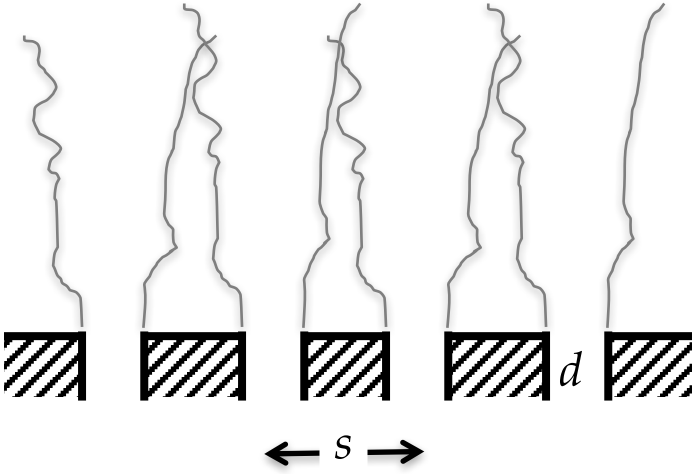
Configuration	*d*, mm	*S*, mm
1	2	--
2	2	6.35
3	0.8	3.5

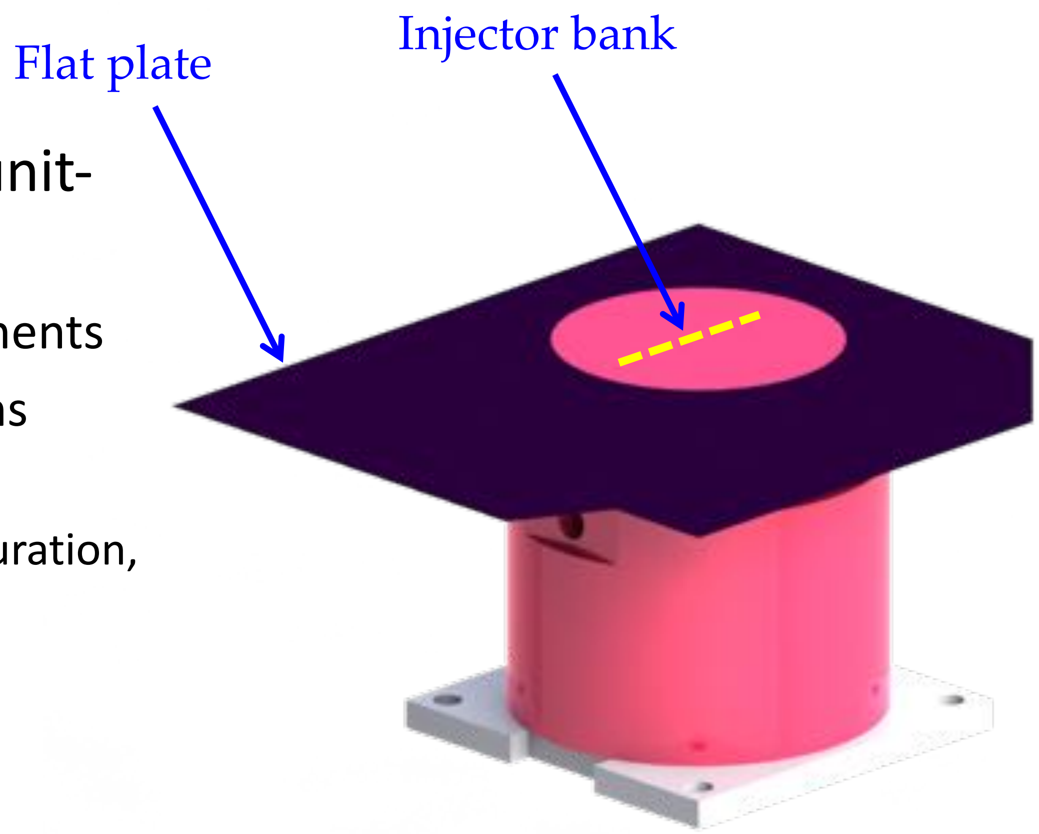


Note: non-reacting cases

Shock-induced mixing in turbulent jets

- Flexible configuration
  - Single isolated injector
  - Multiple isolated injectors

- Well-suited for controlled unit-physics experiments
  - Quantitative mixing measurements
  - Flexibility in range of conditions
    - Shock strength
    - Injection details (speed, configuration, molecular weight)



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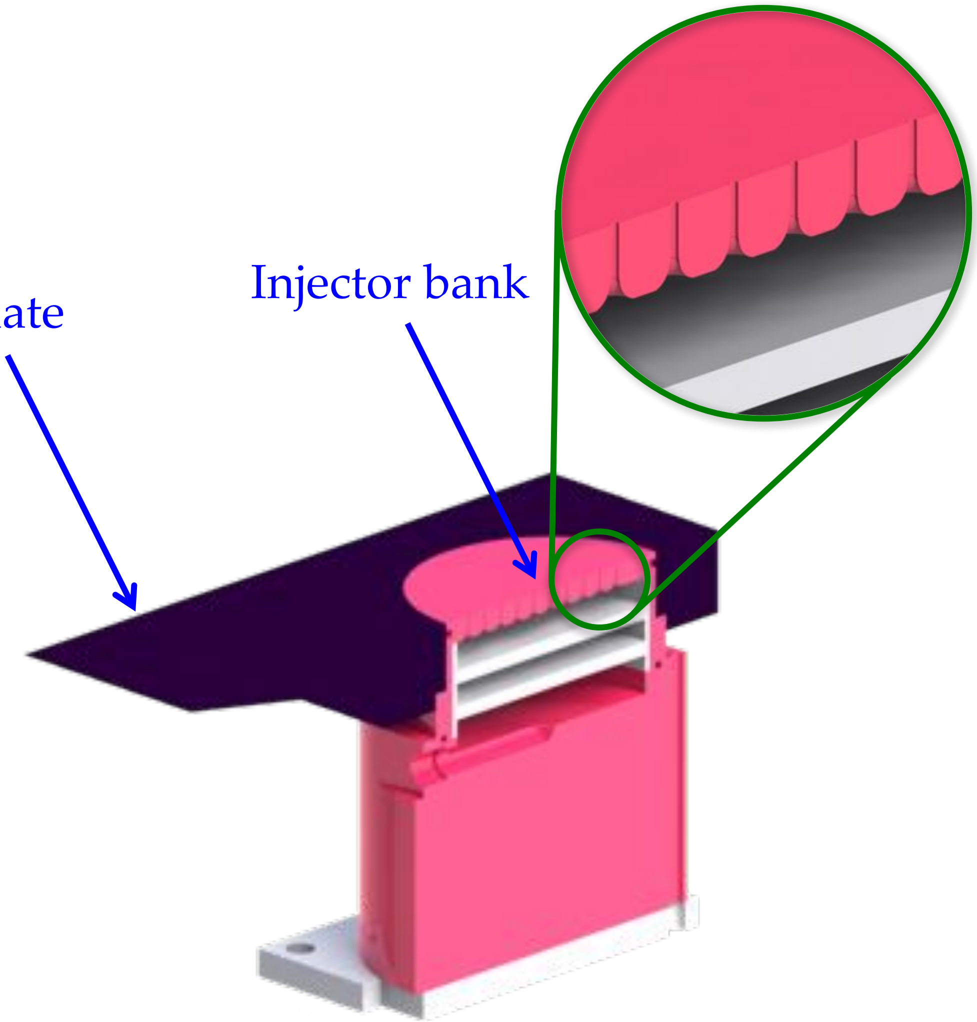
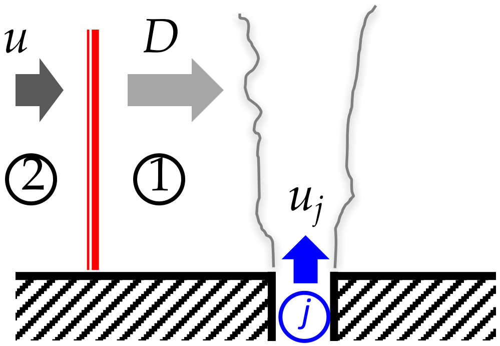
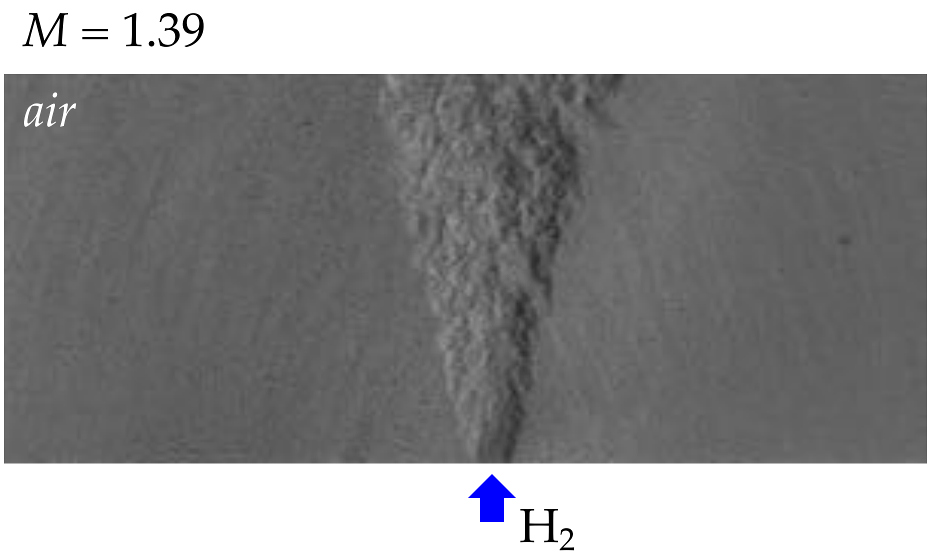


Shock tube facility

Interaction of shock wave with turbulent jet





- Detonation-induced mixing analogue
- Visualization data
  - 100 kHz movie with 300 ns exposure (shock smears by 0.13 pixel)
  - Injection of H_2 into still air subject to a Mach 1.39 shock wave
  - Played back at 5 frames/second
  - Elapsed time 0.5 ms (50 frames)

From initial work presented at UTSR 2015 Workshop

Interaction of shock wave with turbulent jet

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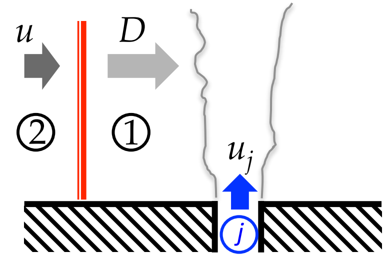

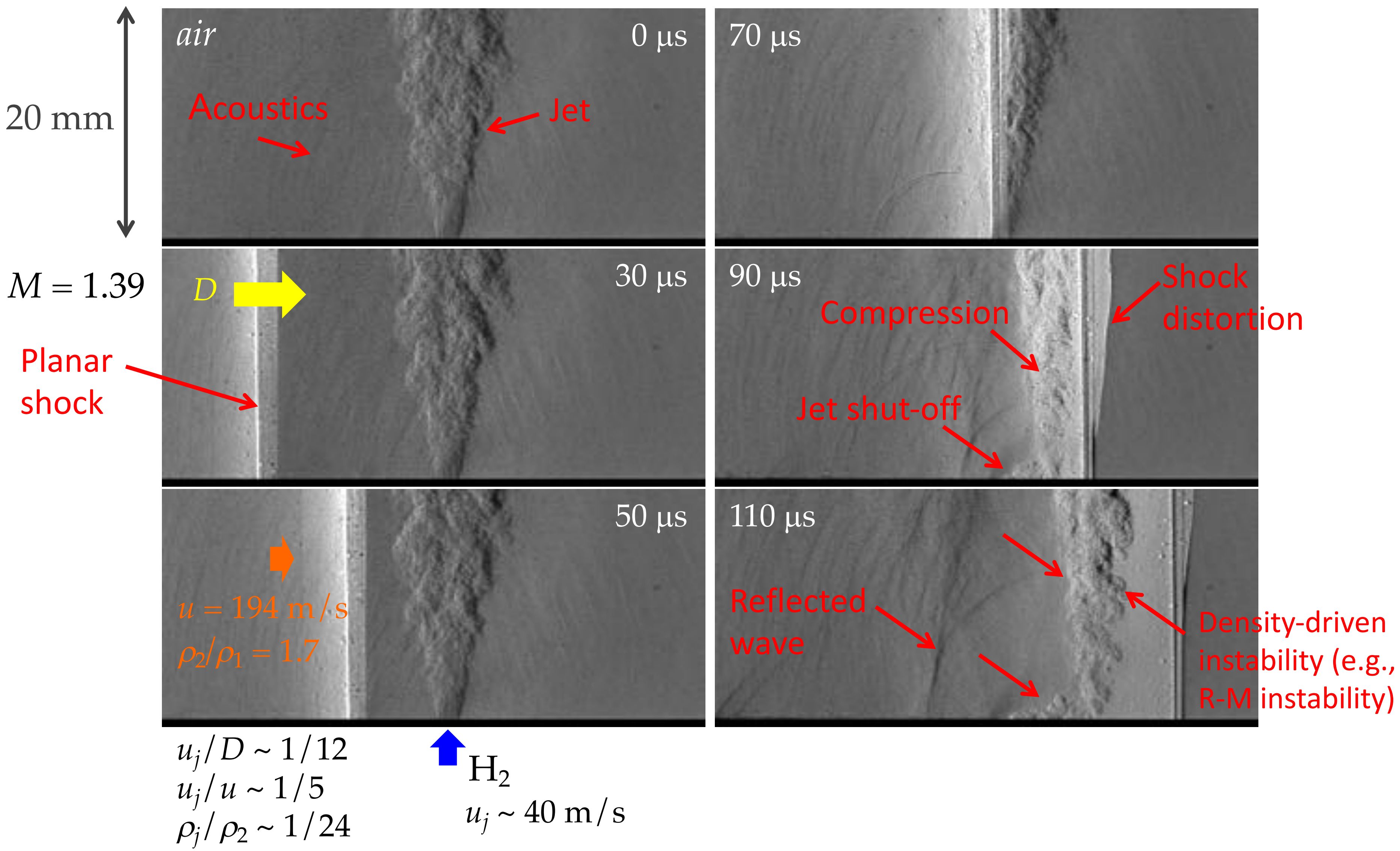

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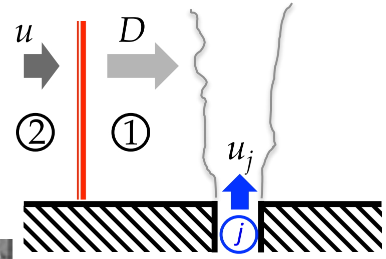
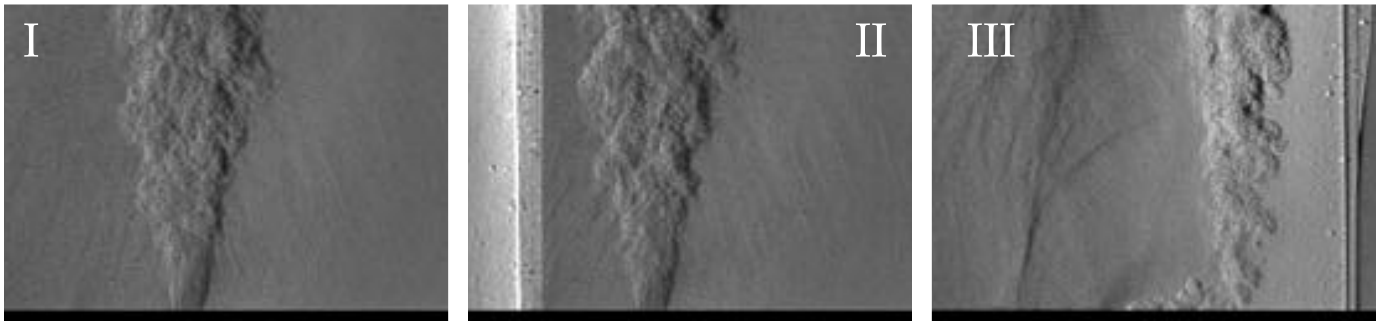
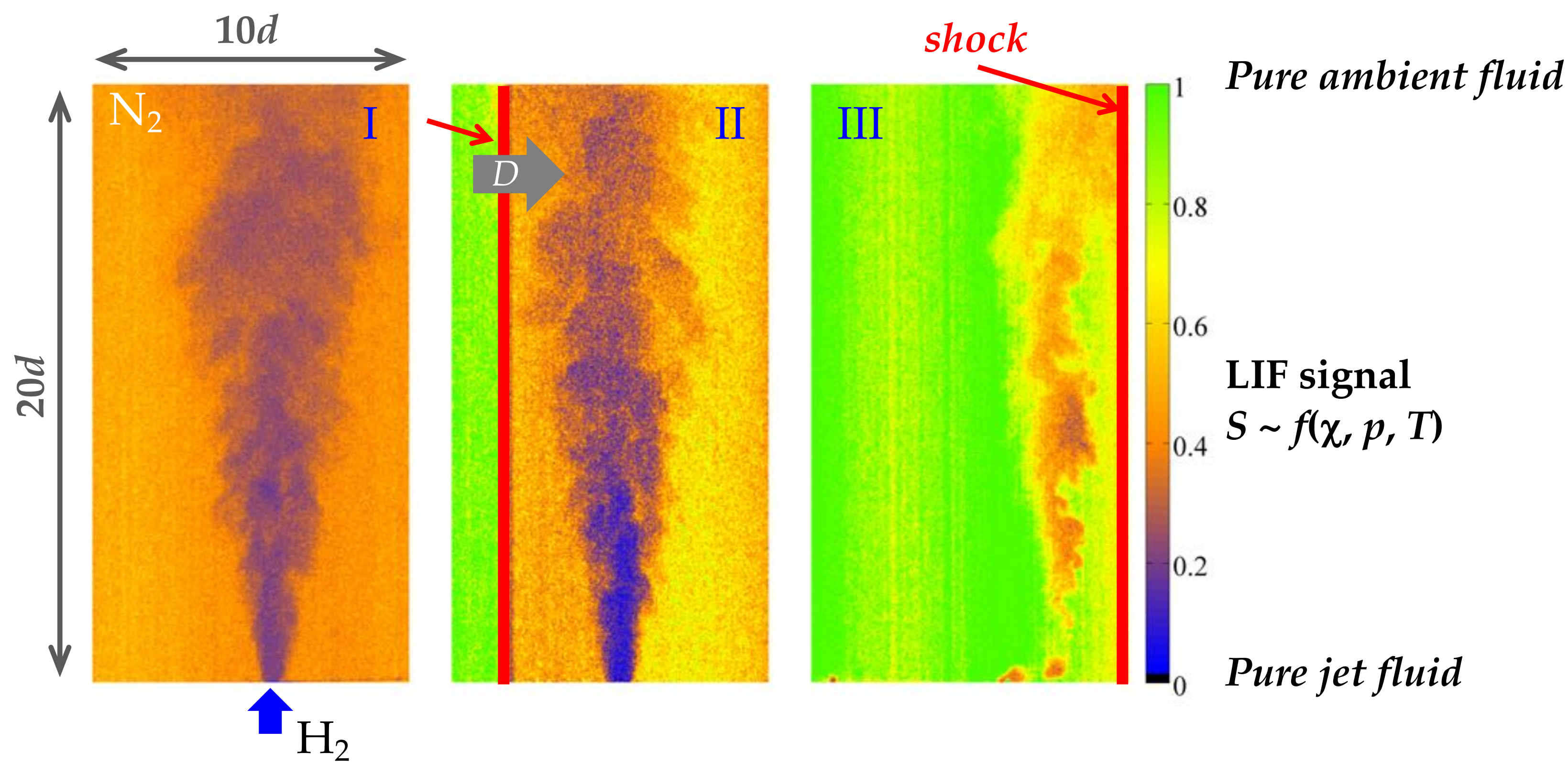
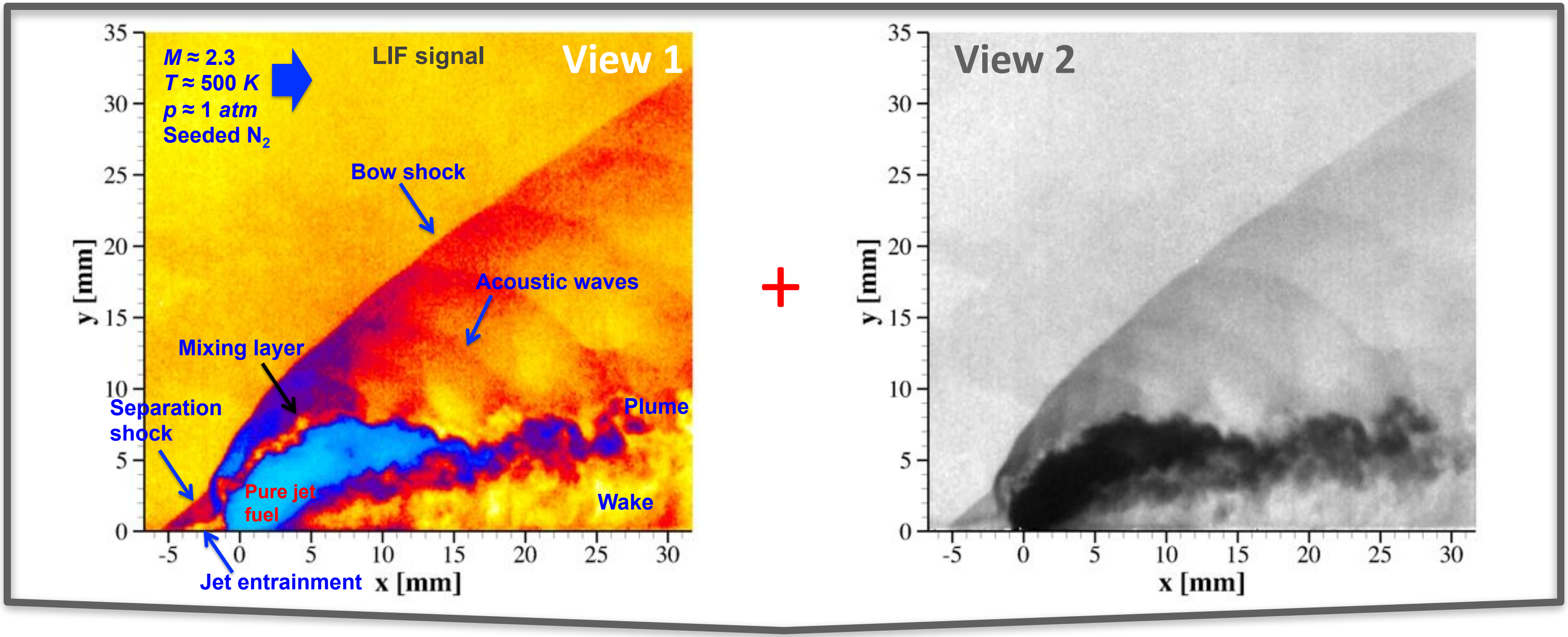


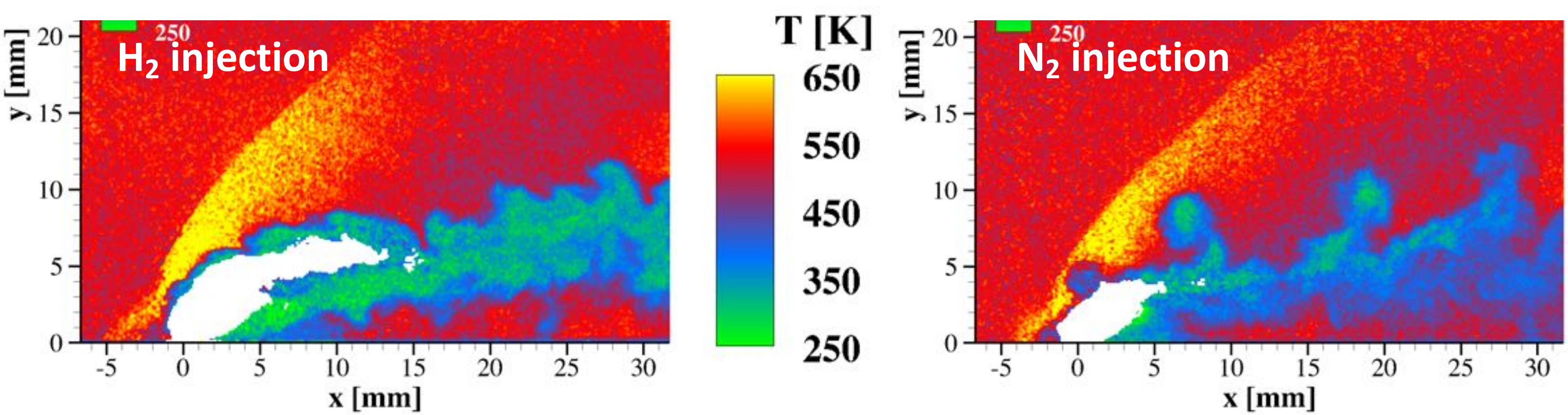




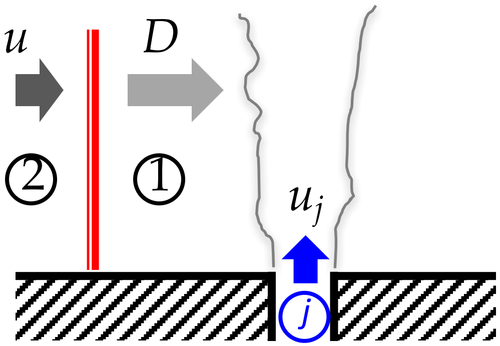
Example of diagnostic application: Making LIF measurements quantitative

Study of transverse jets in supersonic crossflow – non-reacting mixing using toluene PLIF thermometry

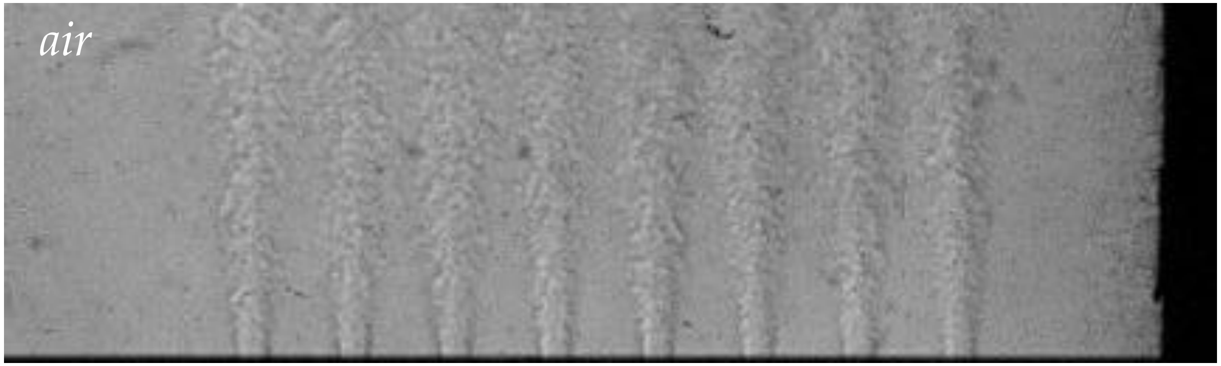




Interaction of shock wave with multiple turbulent jet



Case B1-2: $M = 1.4$



CH_4

- Detonation-induced mixing analogue
- Visualization data
  - 82 kHz movie with 300 ns exposure (shock smears by 0.13 pixel)
  - Injection into still air subject to a shock wave
  - Played back at 5 frames/second
  - Elapsed time 0.5 ms (50 frames)

Strong jet density variation

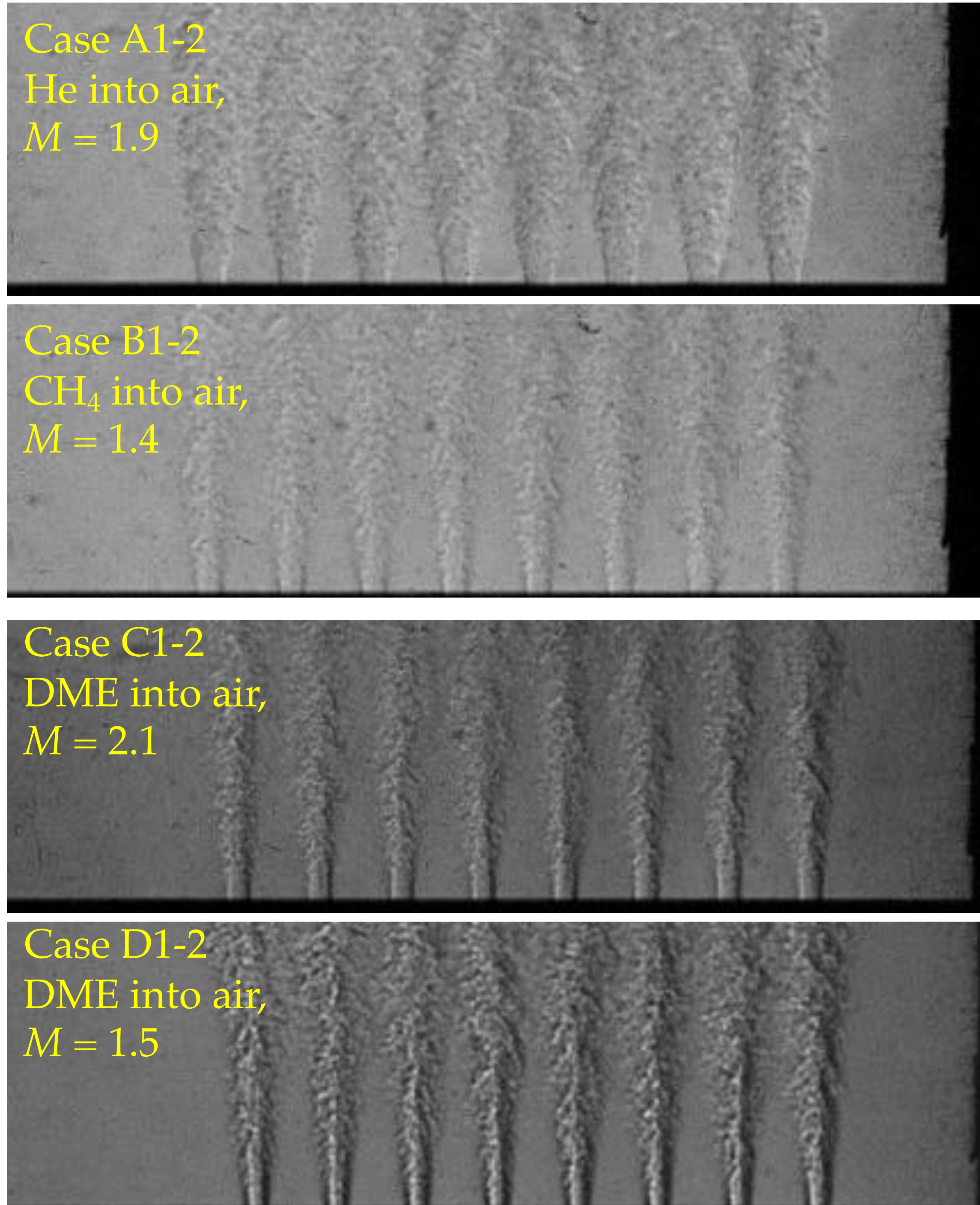
Impact on:

- Shock propagation speed across jets
- Shock front curvature

Shock strength variation

Impact on:

- Jets compression
- Jets instabilities
- Jets structure and scale orientation
- Mixing



Strong jet density variation

Impact on:

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Shock strength variation

Impact on:

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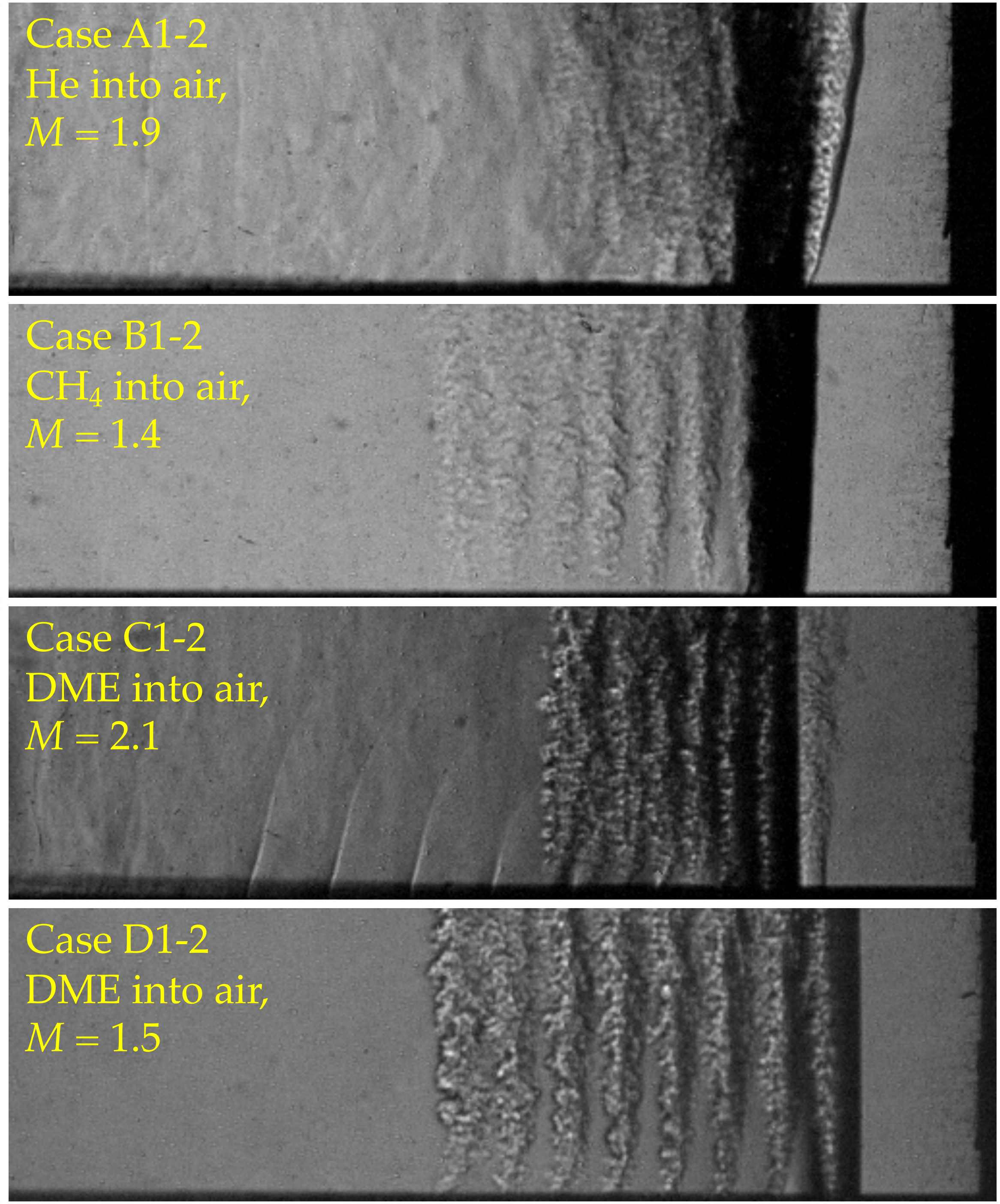
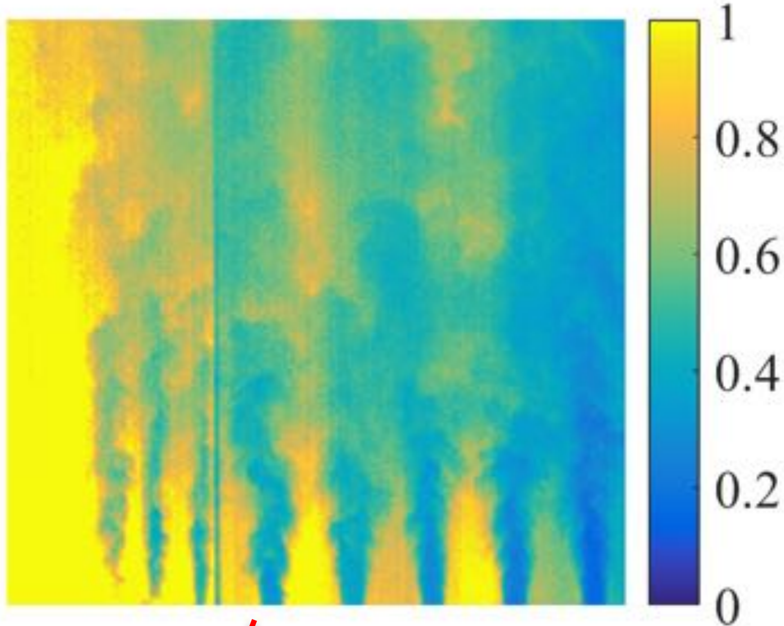
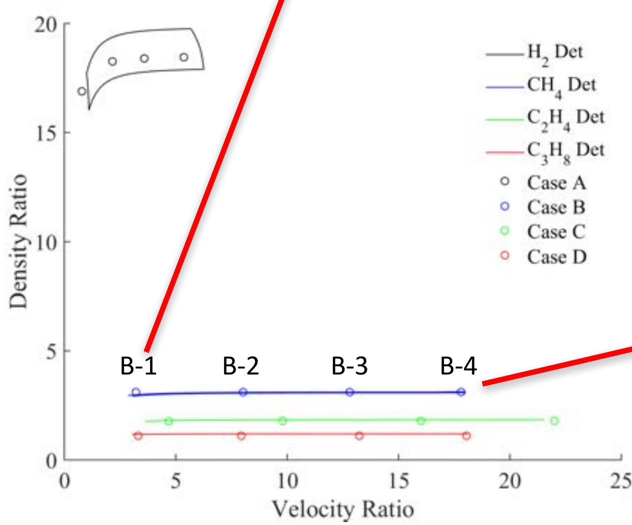
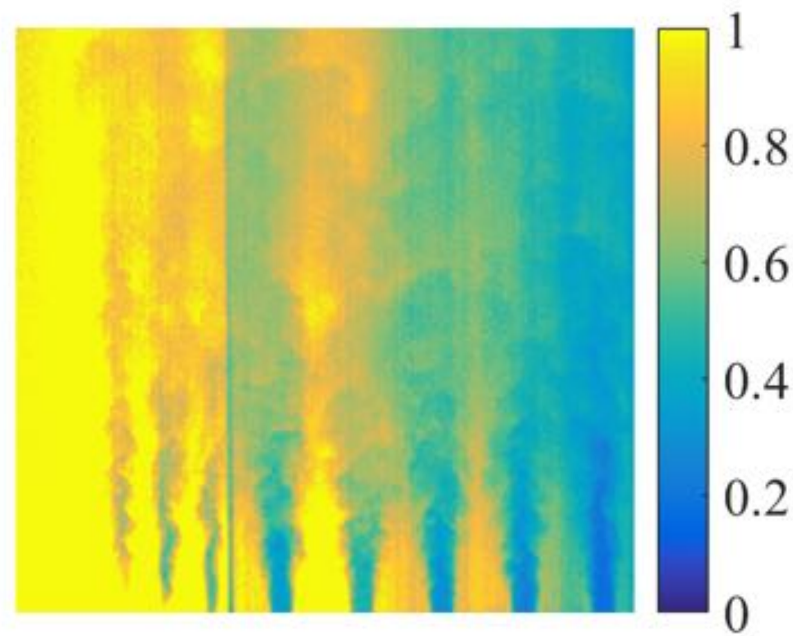


Ongoing work on interaction of shock wave with turbulent jet array: Mixing study using tracer PLIF

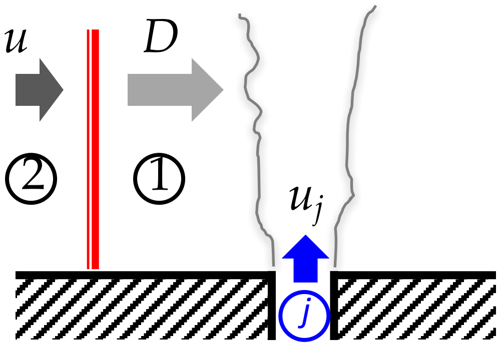


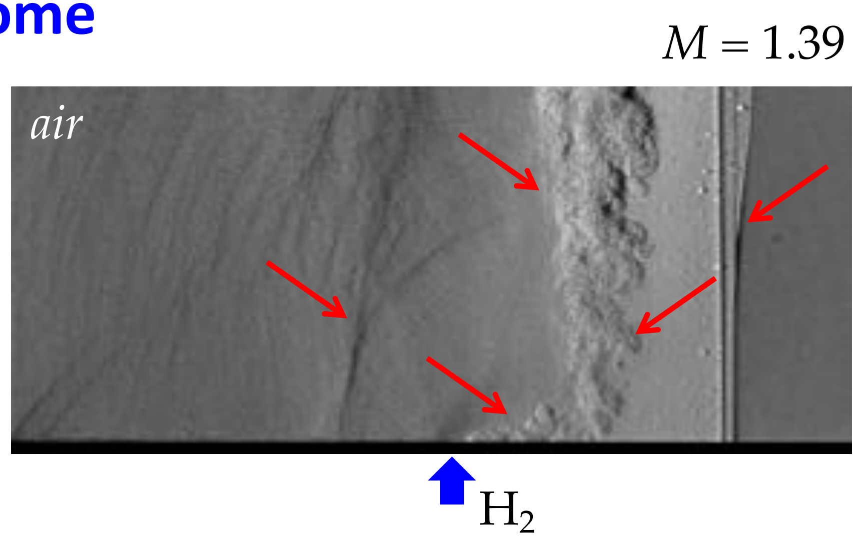
- Shown is a qualitative flow visualization
- Nearly the same density ratio, but case B-4 has 4x the velocity ratio of case B-1
- Velocity ratio affects post-shock mixing field
  - More rapid mixing behind the shock wave as velocity ratio increases
  - Why?





Ongoing work on interaction of shock wave with turbulent jet array: Parametric study and outcome





- Parameters to be varied
  - Shock strength (Mach #)
  - Injectant/ambient species
    - Light/heavy vs heavy/light
    - Injectant-to-ambient density and velocity ratios
    - Injection pressure ratios
  - Injection configuration
- Performance metrics
  - Degree of mixing (spatial measurement)
  - Plume shape
    - Width, corrugation, deflection
  - Length and time scales of injector response
  - Scaling with working parameters
    - Density & velocity ratios
    - Plume compression rate
    - Injector size and spacing

Planned experimental multi-level approach

RDE full system:
- Link between mixing and performance
- Design from ISSI/AFRL

Linearized analogue:
- Detonation structure
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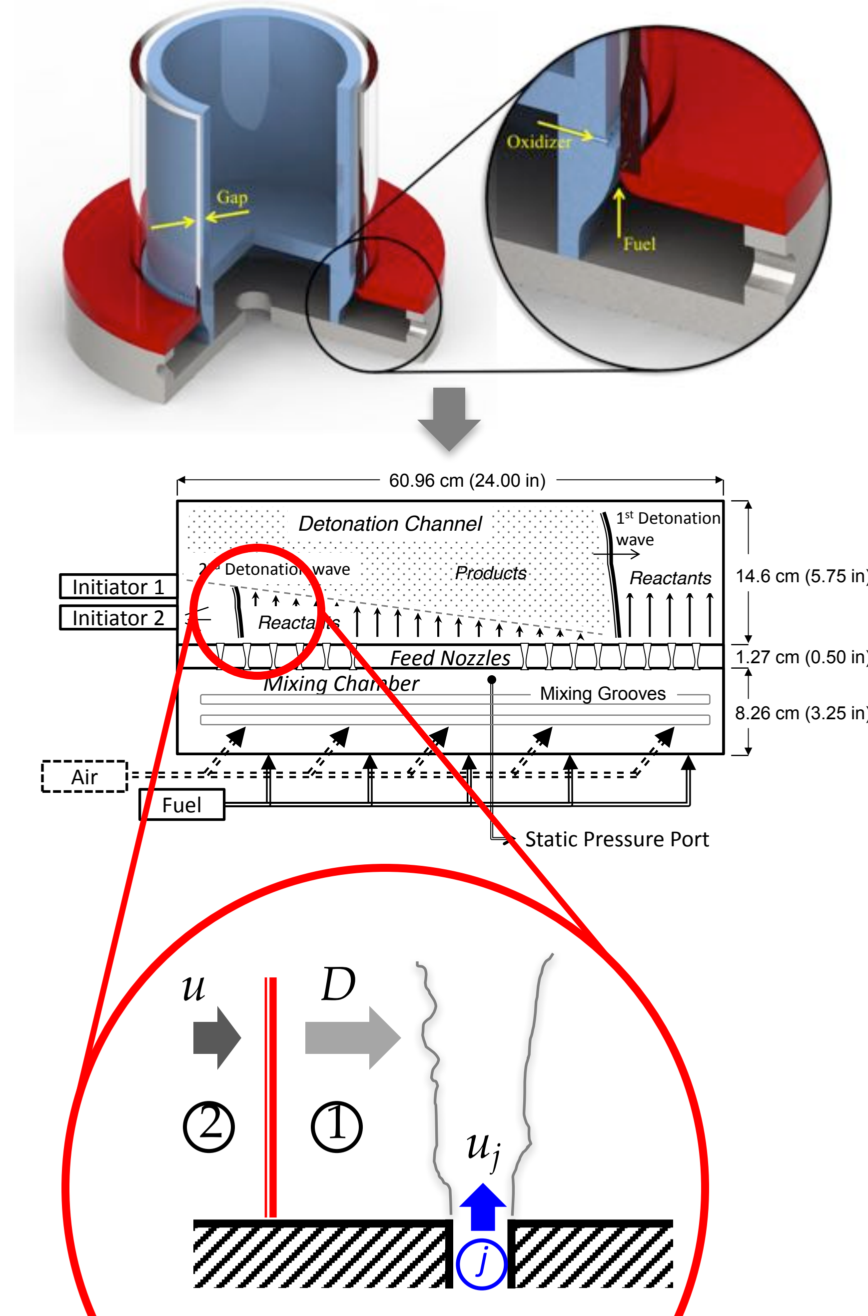
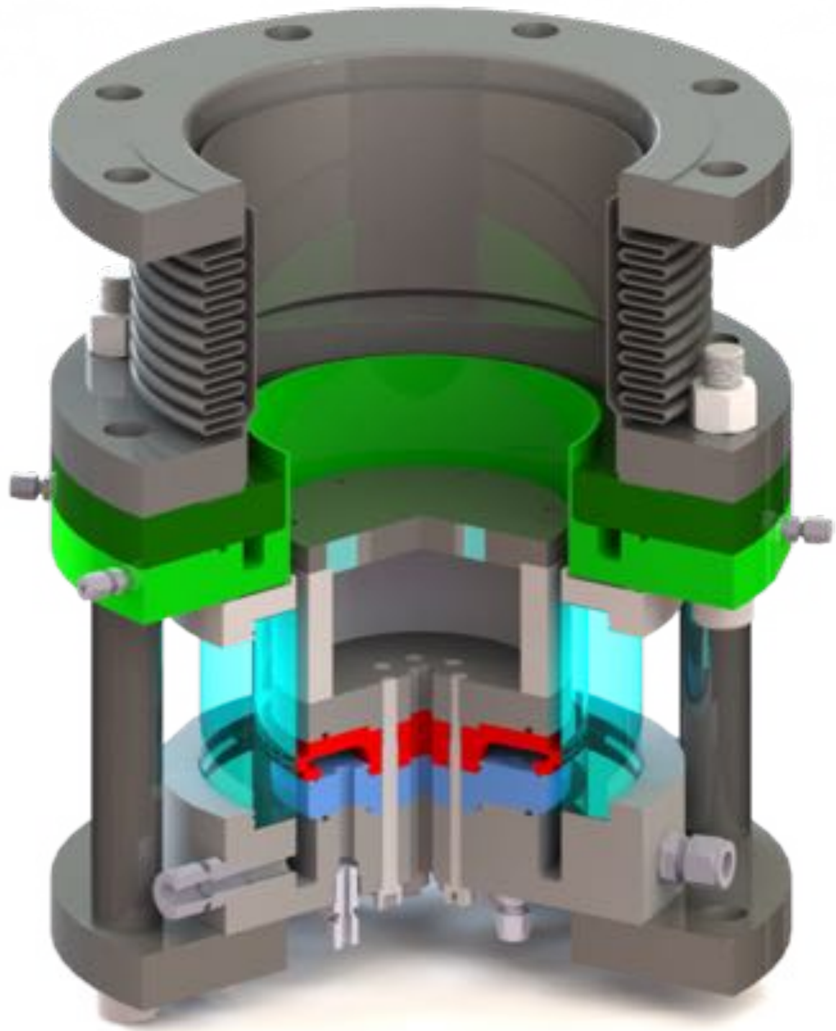
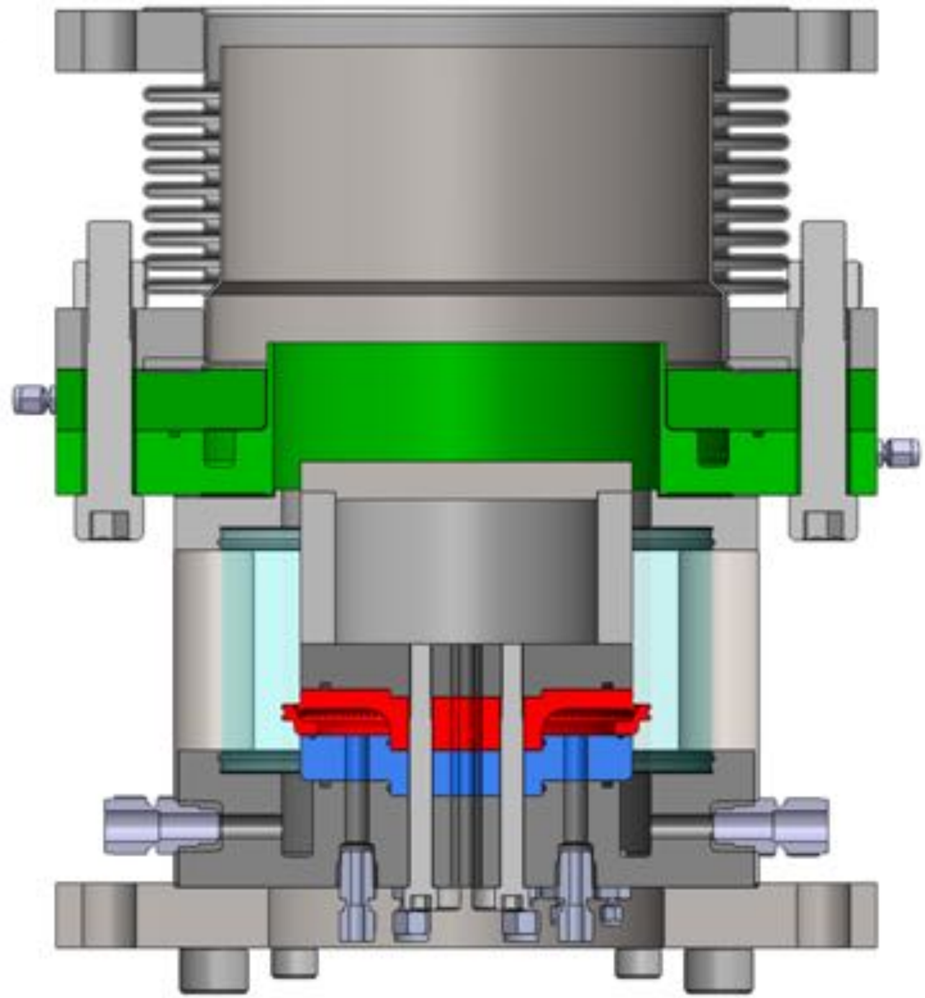
Single or multiple injectors:
- Mixing studies
- Shock-induced mixing
- Our starting point



Hierarchy

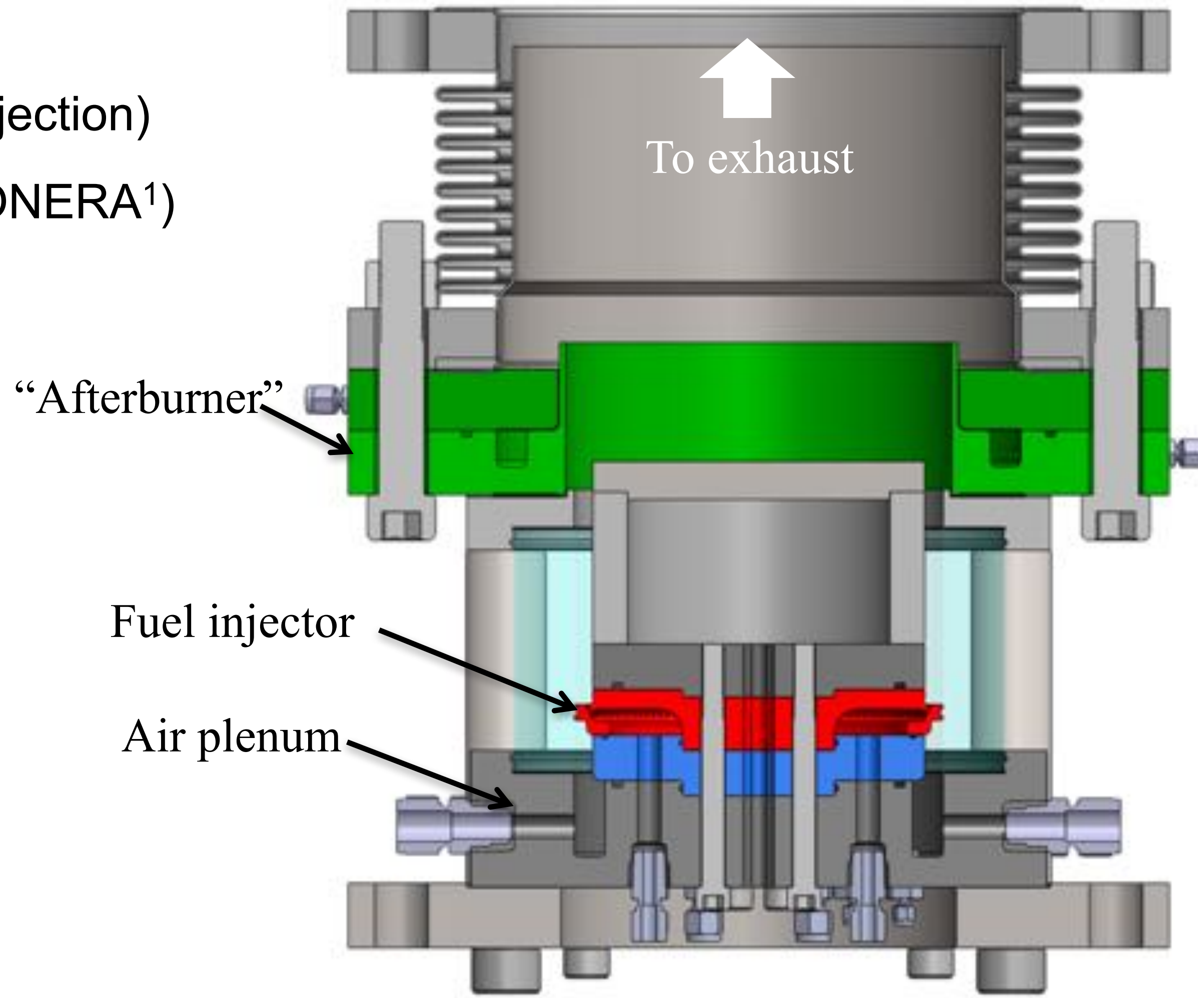
Development of a flexible RDE hardware at U-M





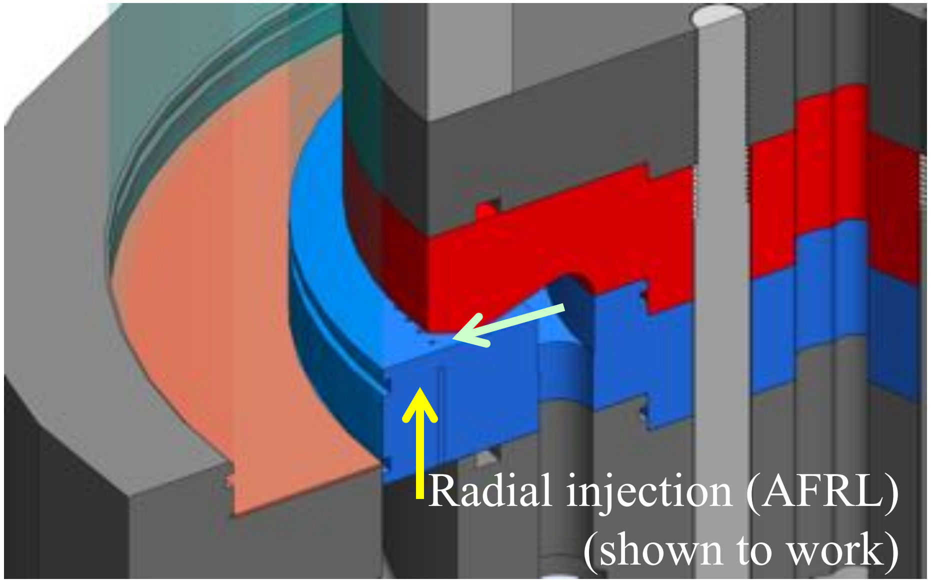
Development of a flexible RDE hardware at U-M

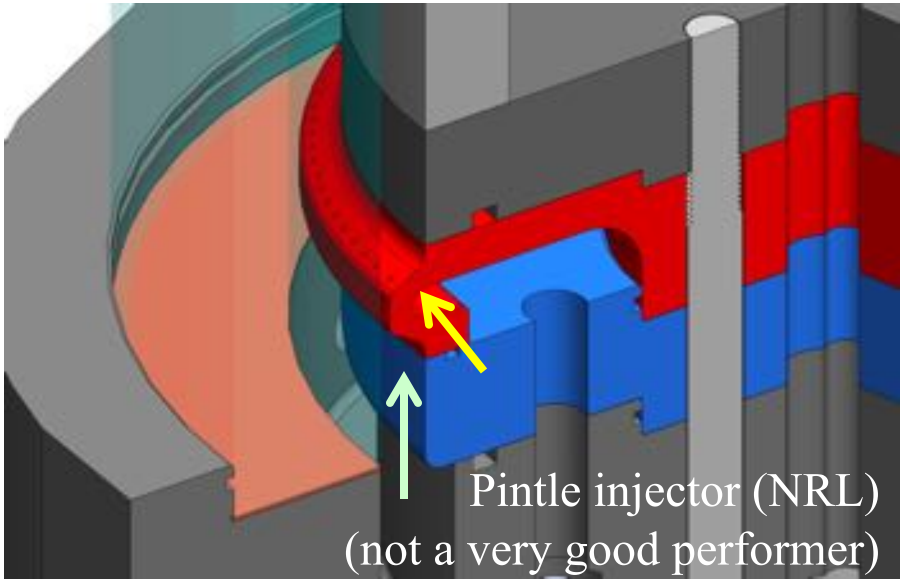
- Modular configuration
- Multiple injection schemes
  - AFRL design (radial injection)
  - Semi-impinging jets (ONERA[1])
  - Pintle injector (NRL[2])

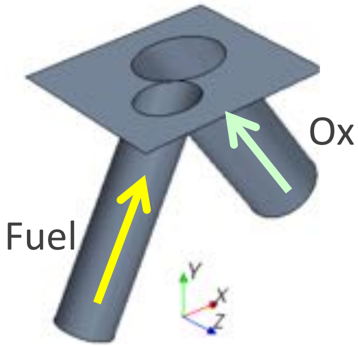


[1] Gaillard et al., Acta Astronautica, 111:334-344 2015
[2] Schwer & Kalaisanath, 2015 AIAA Scitech, AIAA-2015-3782

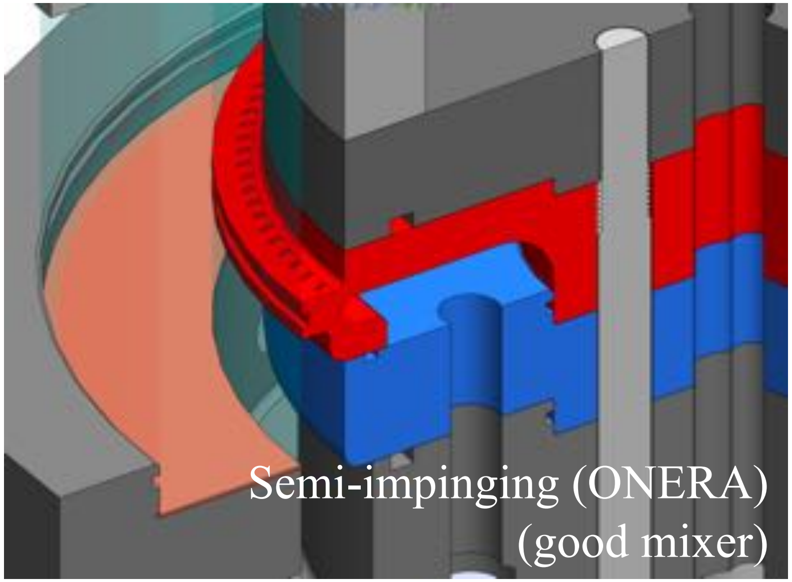
Development of a flexible RDE hardware at U-M

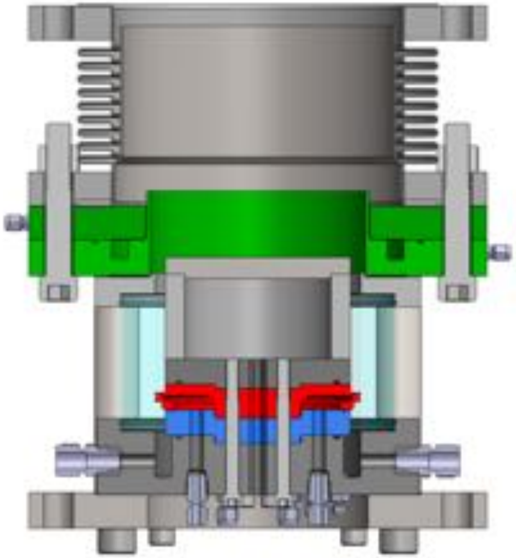




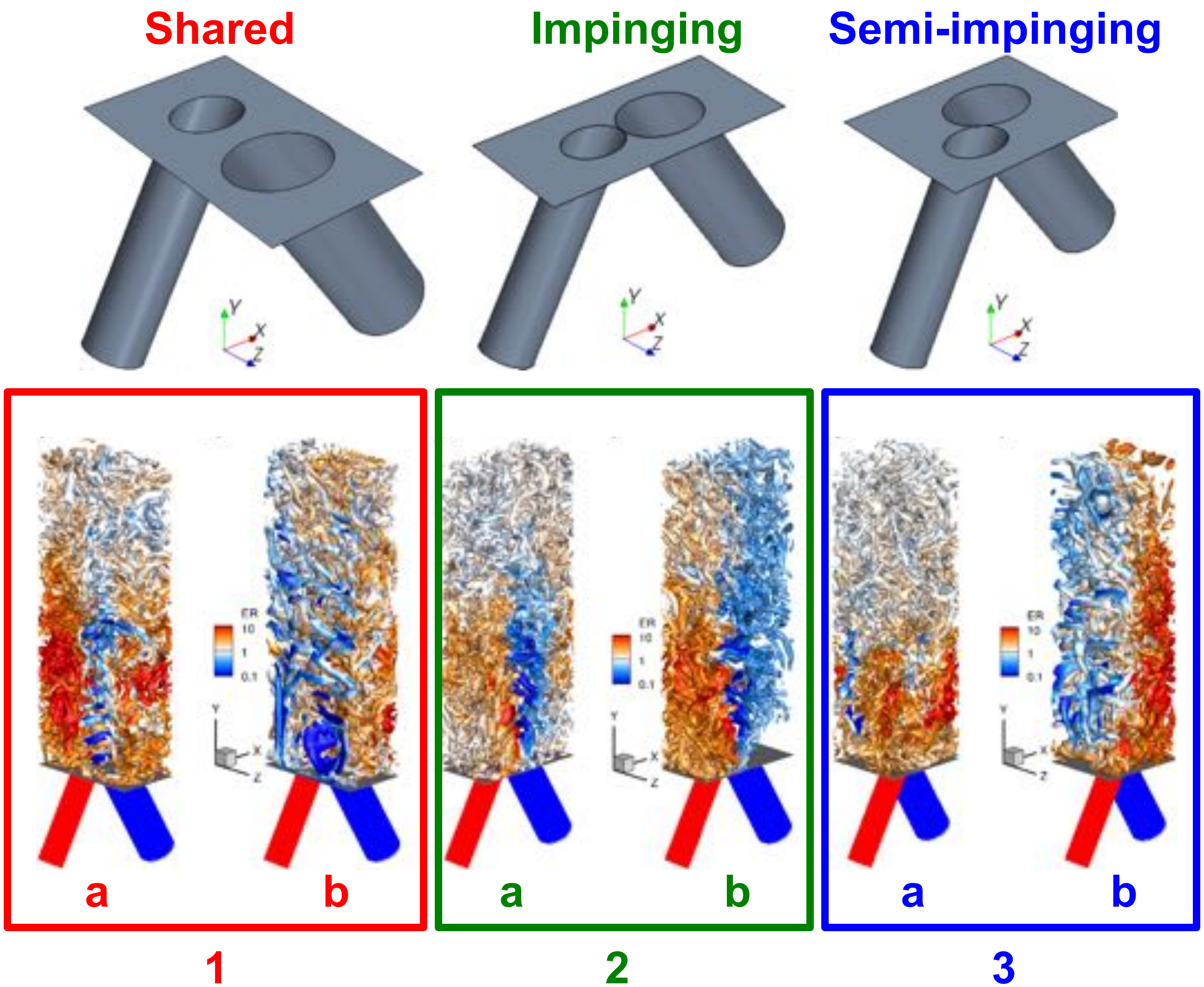


From Gaillard et al., Acta Astronautica, 111:334-344 2015





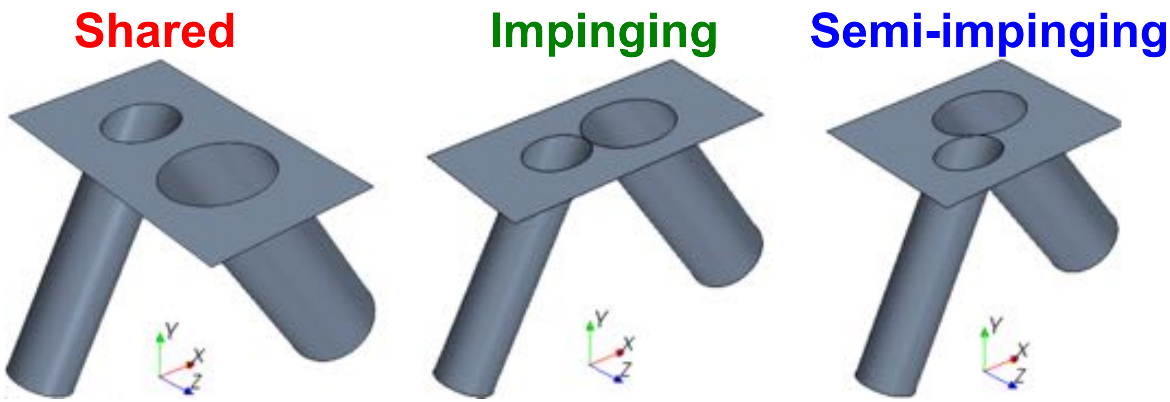
Gaillard et al. (2015) evaluated different jet configurations

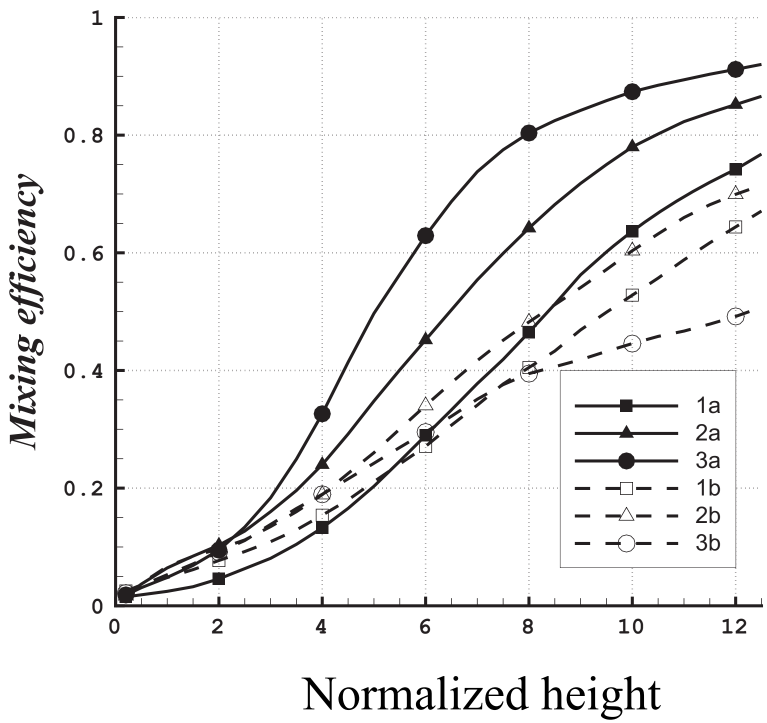


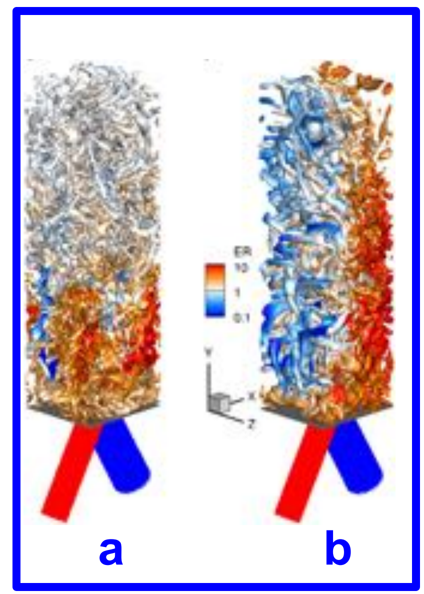
a: periodic
b: symmetric

From Gaillard et al., Acta Astronautica, 111:334-344 2015

Gaillard et al. (2015) evaluated different jet configurations







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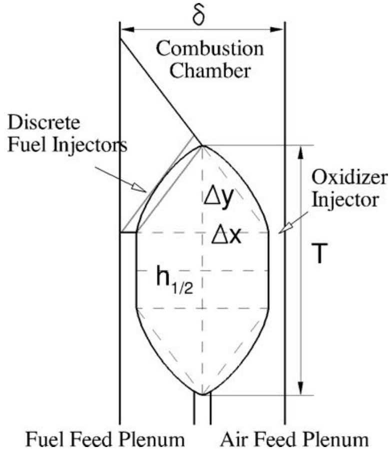
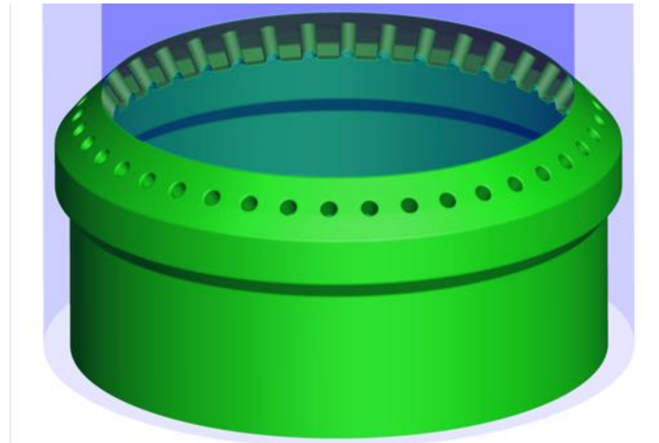
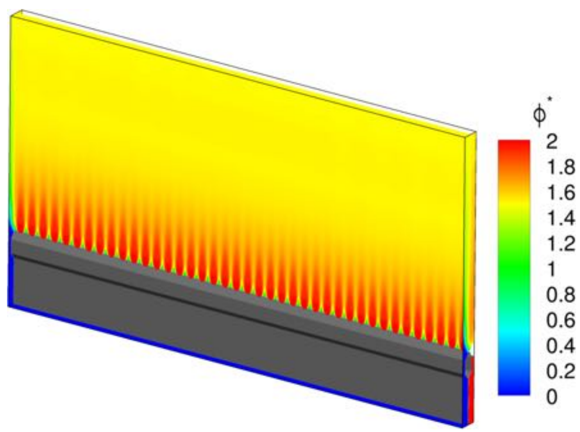
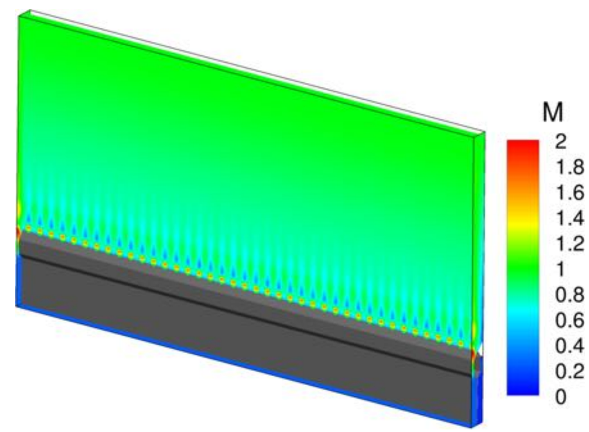
From Gaillard et al., Acta Astronautica, 111:334-344 2015

Schwer & Kailasanath evaluated a pintle-like design





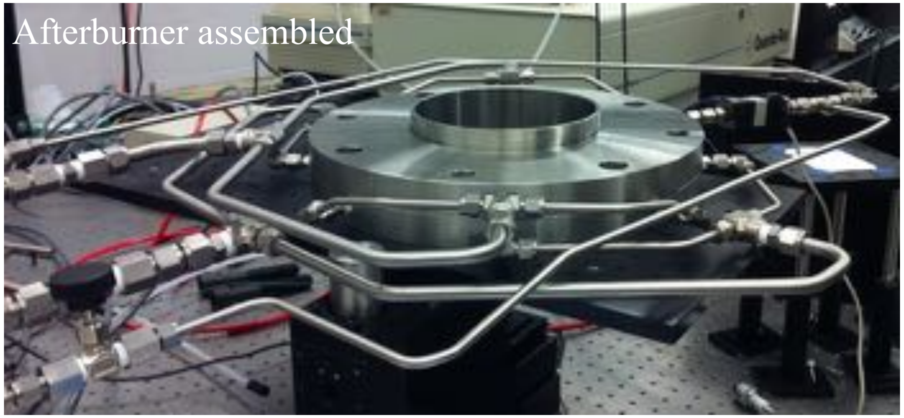


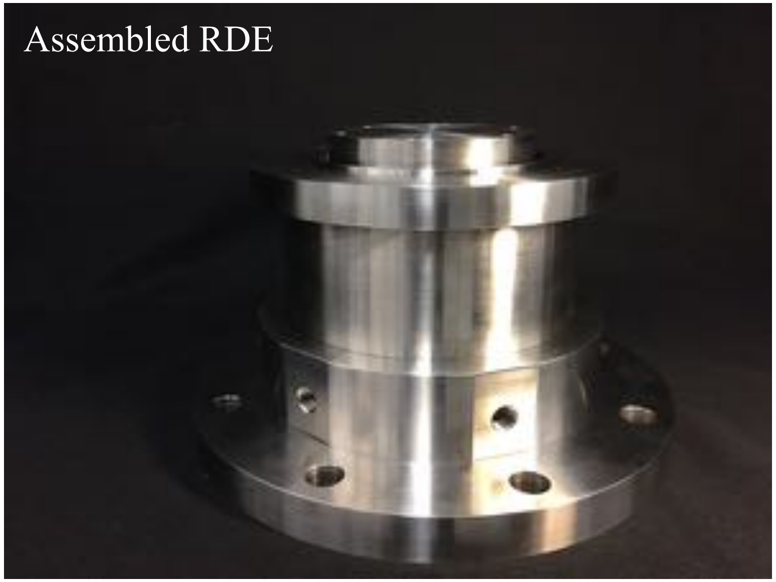


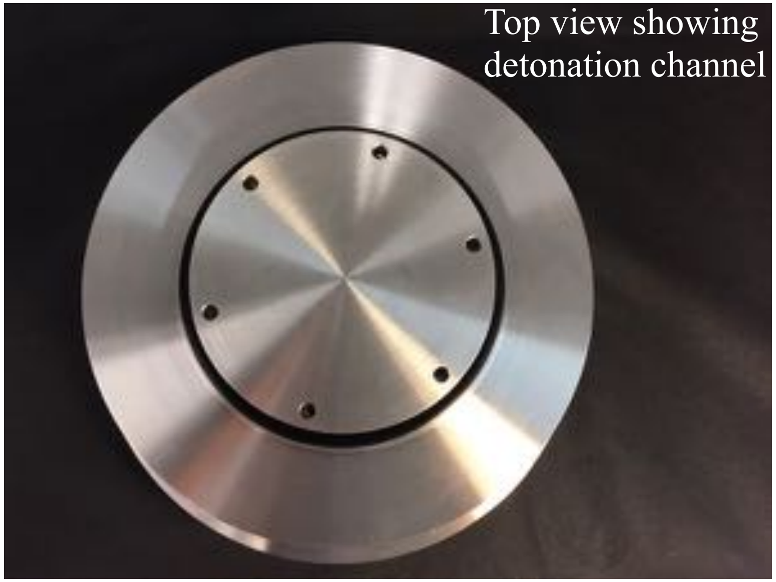
- Azimuthal stratification
- Detonation could not be stabilized

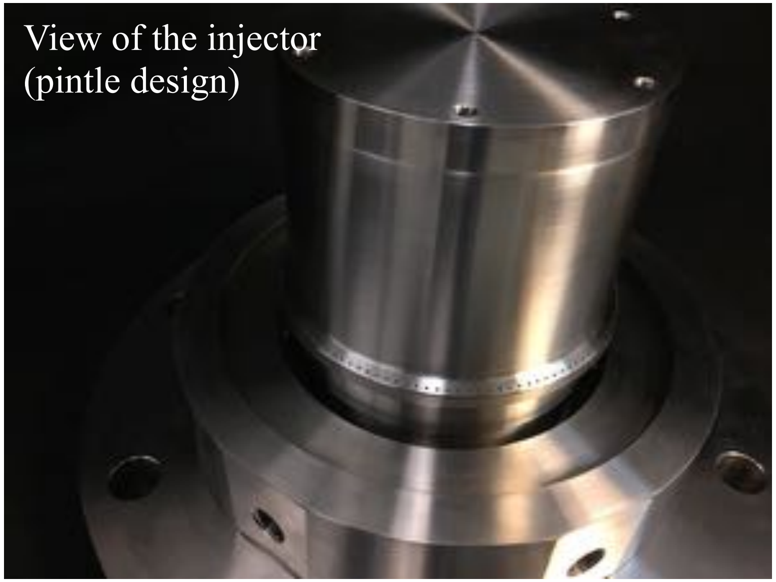
Schwer & Kalaisanath, 2015 AIAA Scitech, AIAA-2015-3782

Flexible RDE hardware (Round RDE)







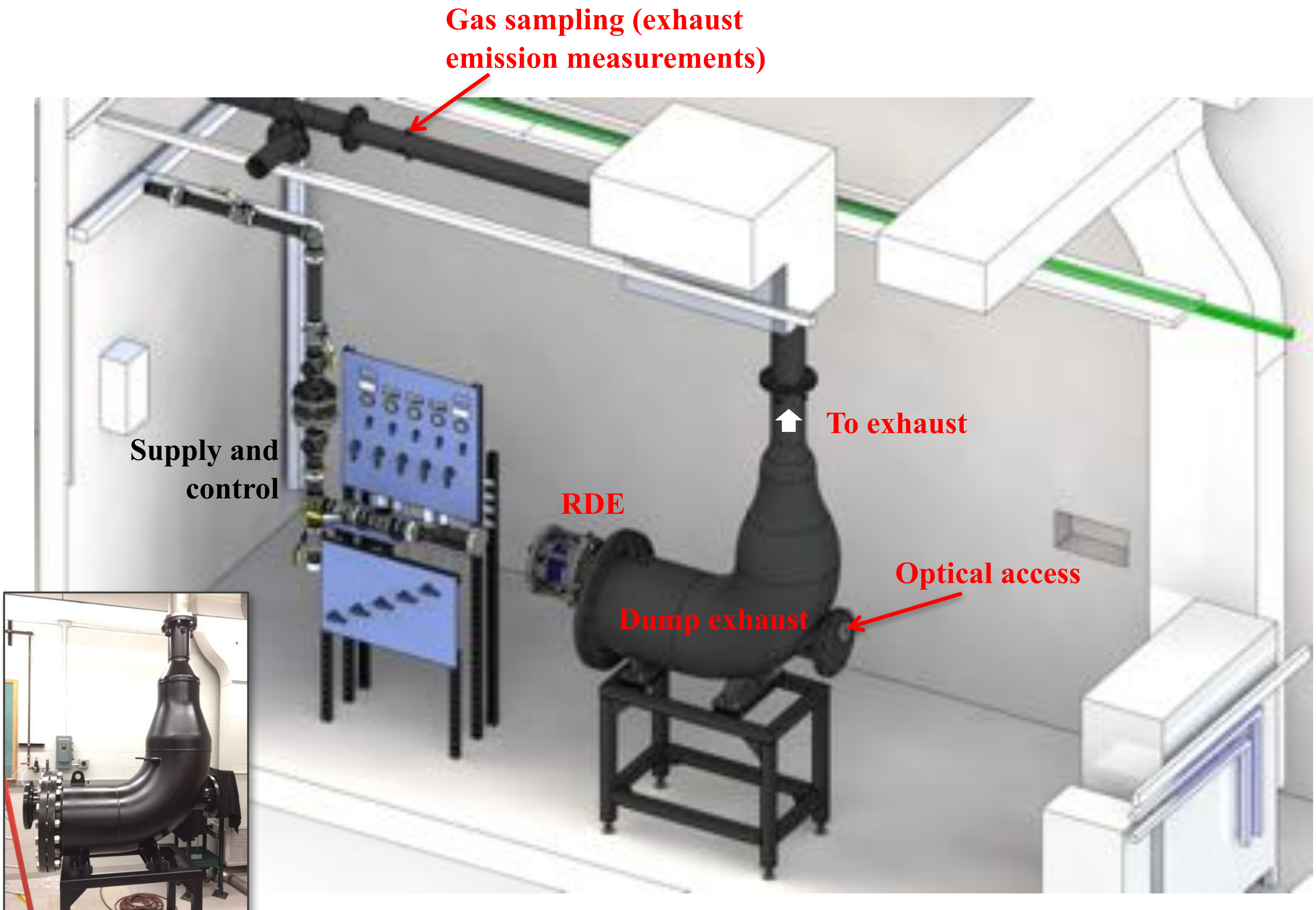


Testing of the afterburner

Next steps on the development of RDE system

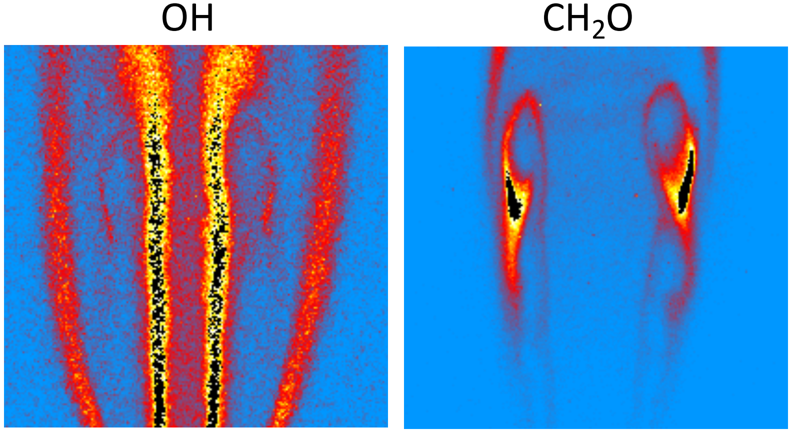
- Evaluate flow properties (non-reacting) produced by RDE
- Integration of RDE with exhaust, supply and control systems
- Testing of integration, control system and test sequence under unfueled operation
- Testing under fueled operation

How it will look like after integration is completed



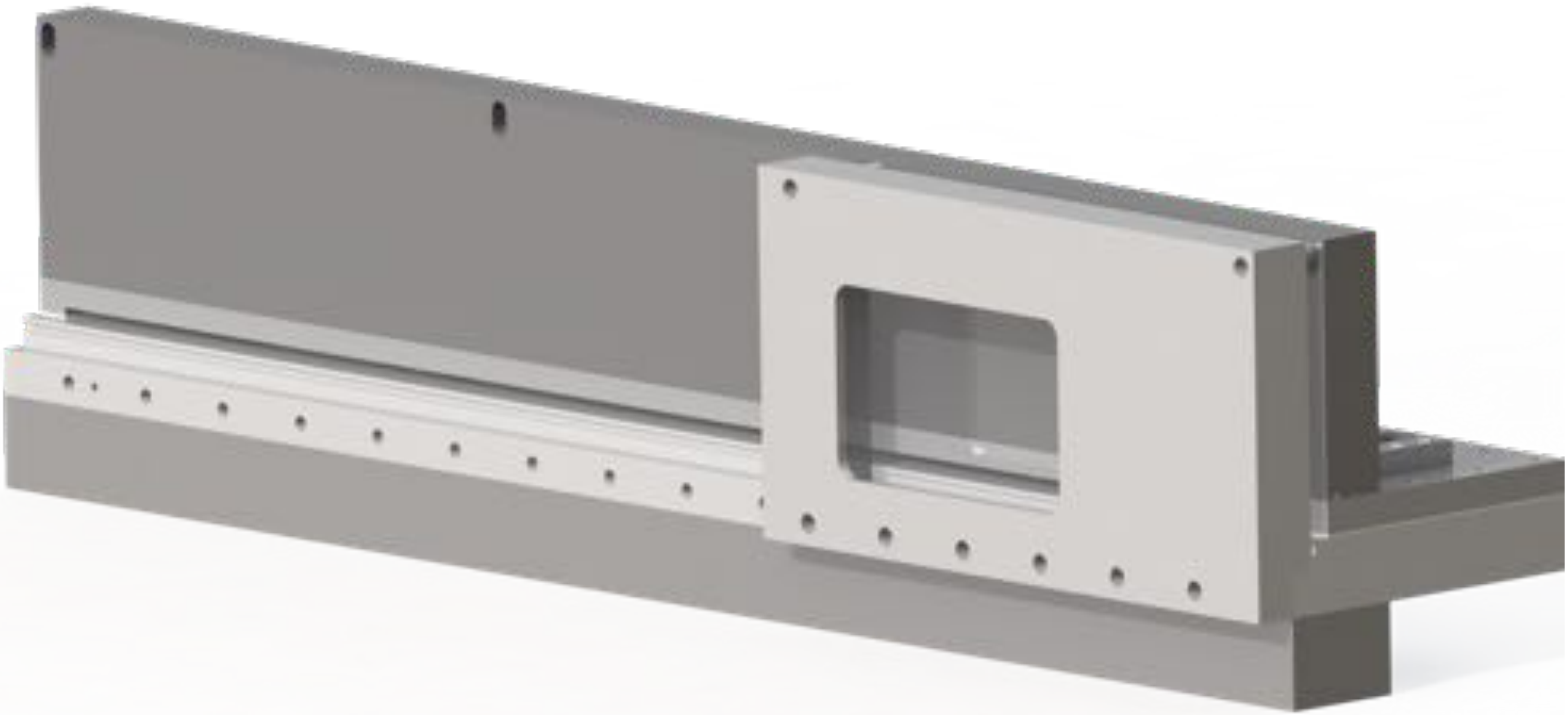
Planned suite of diagnostic techniques for the study of RDE physics

- Traditional techniques:
  - Pressure, heat flux, flame chemiluminescence
  - Schlieren imaging
- Laser-based imaging diagnostics:
  - Planar laser-induced fluorescence (PLIF) mixing and flame marker
  - Two-color toluene PLIF thermometry and mixing (non-reacting) imaging
  - OH/CH_2O/CH/NO PLIF imaging
    - e.g., Simultaneous OH/CH_2O PLIF imaging for flame structure and heat release distribution study in premixed combustion
  - Rayleigh scattering imaging (thermometry in reacting flows)
- But we need an optically accessible system



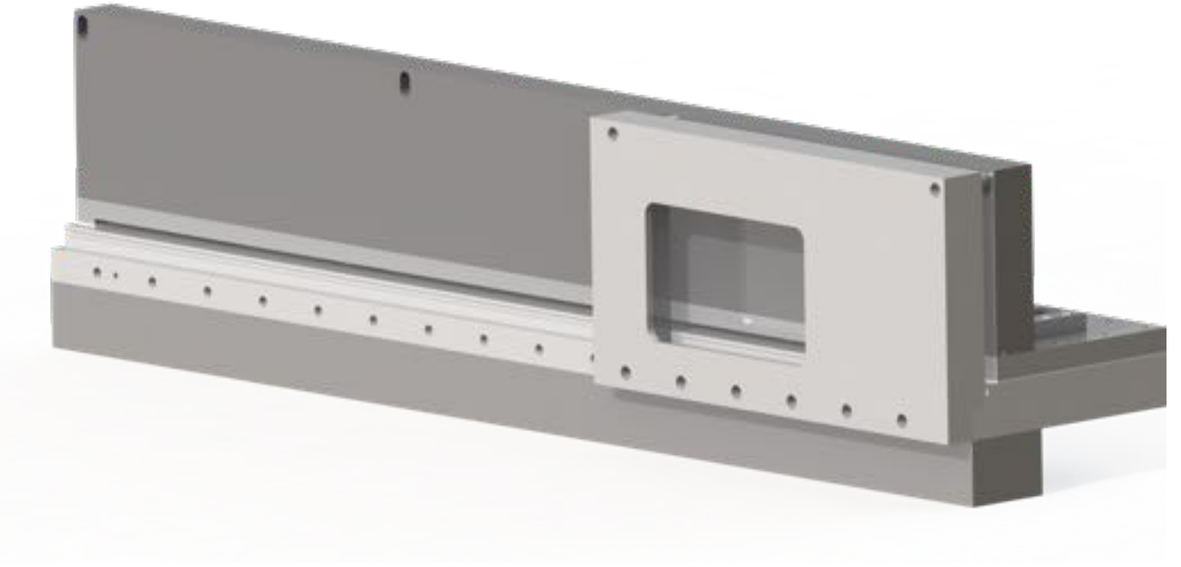
Simultaneous OH/CH_2O PLIF imaging in inverted oxy-fuel coaxial non-premixed CH_4 flames

Development of linearized RDE (what originally planned)



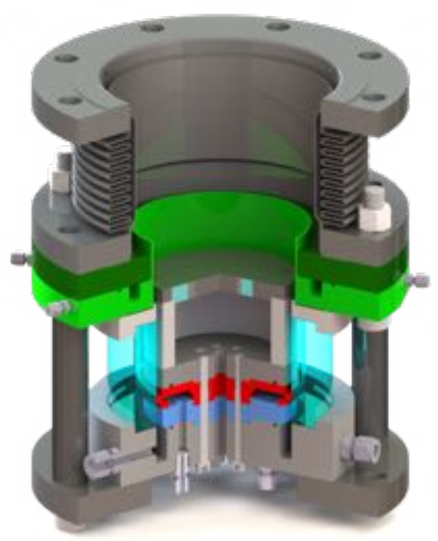
- Designed after AFRL design (radial injection)
- Pre-detonator to generate a planar detonation designed
- Designed, but not built yet

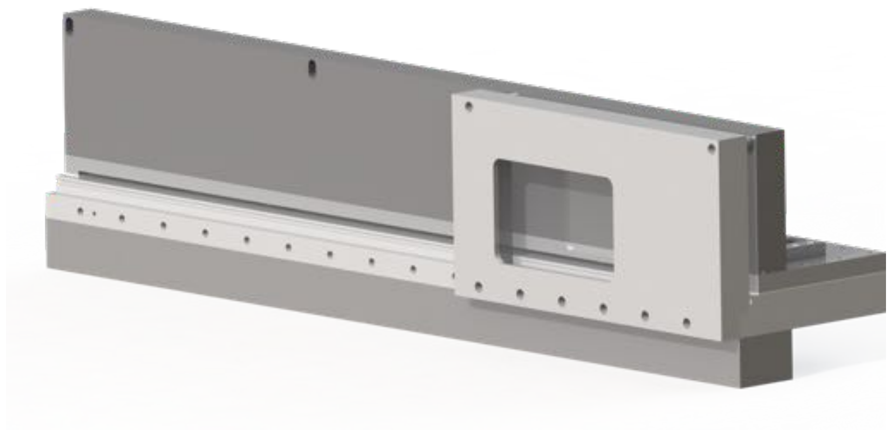
Development of linearized RDE (what originally planned)



- **Benefits**
  - Simple configuration to study and model
  - Allows for optical access for laser diagnostics
- **Drawbacks**
  - Intermittent operation (2 or 3 detonation cycle)
  - Unclear if a fully-developed detonation wave can be achieved (due to limited length and intermittent operation)
  - May not allow to reach stationary parasitic combustion

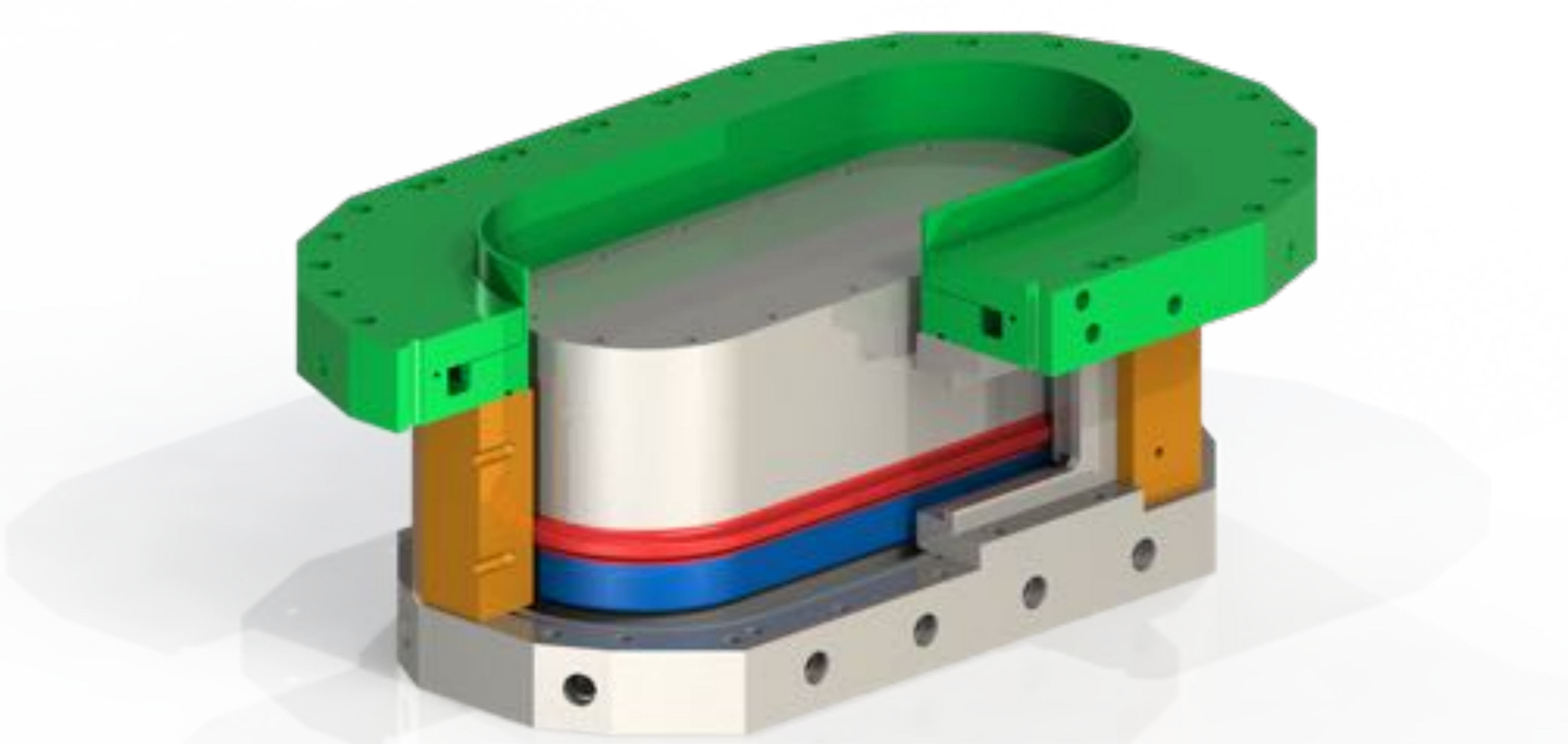
Proposed hybrid RDE



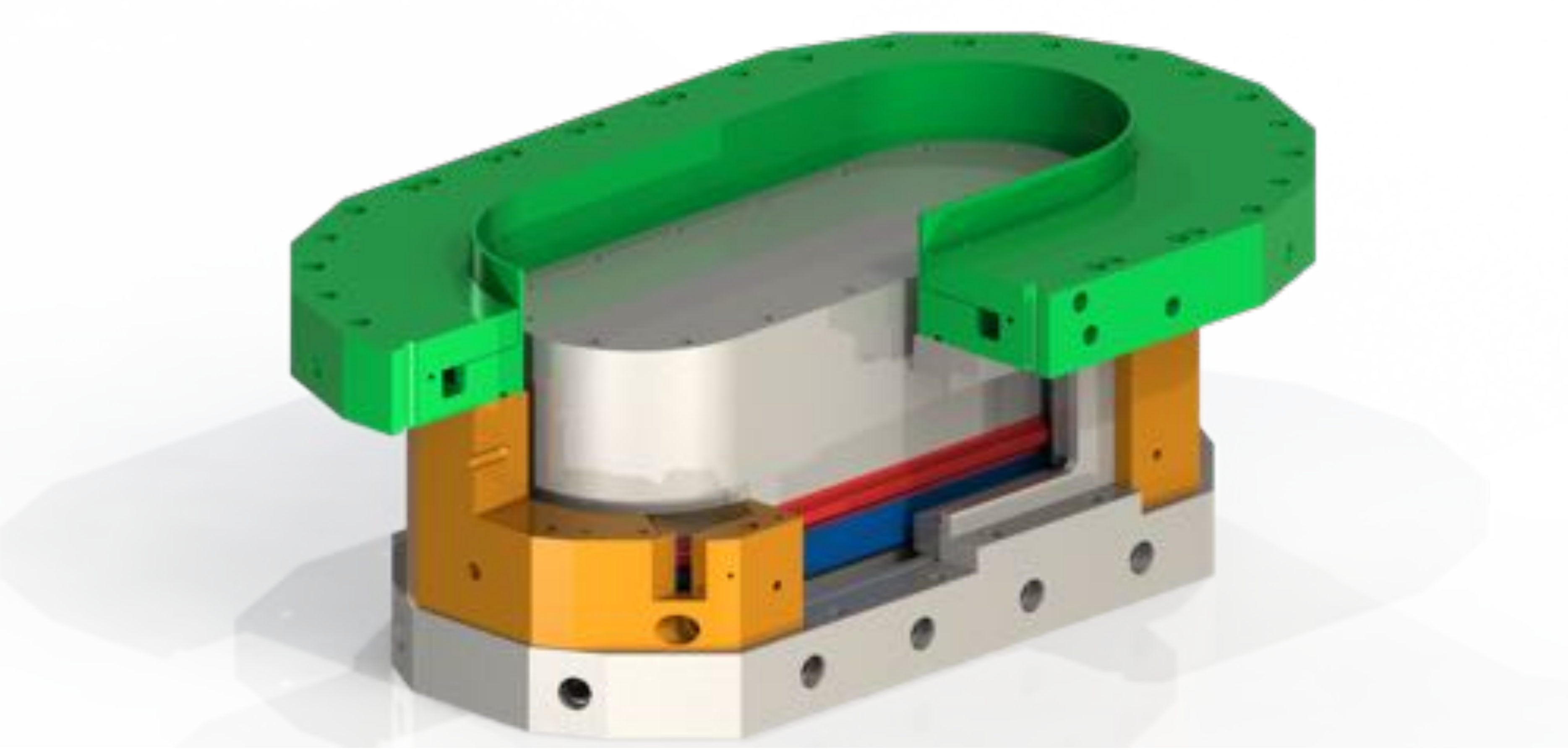


- Designed with features similar to our RDE configuration
- Feasibility design study almost completed
  - Awaiting verification of optical components

Proposed Hybrid RDE (Race Track RDE, or RT-RDE)



Proposed Hybrid RDE (Race Track RDE, or RT-RDE)



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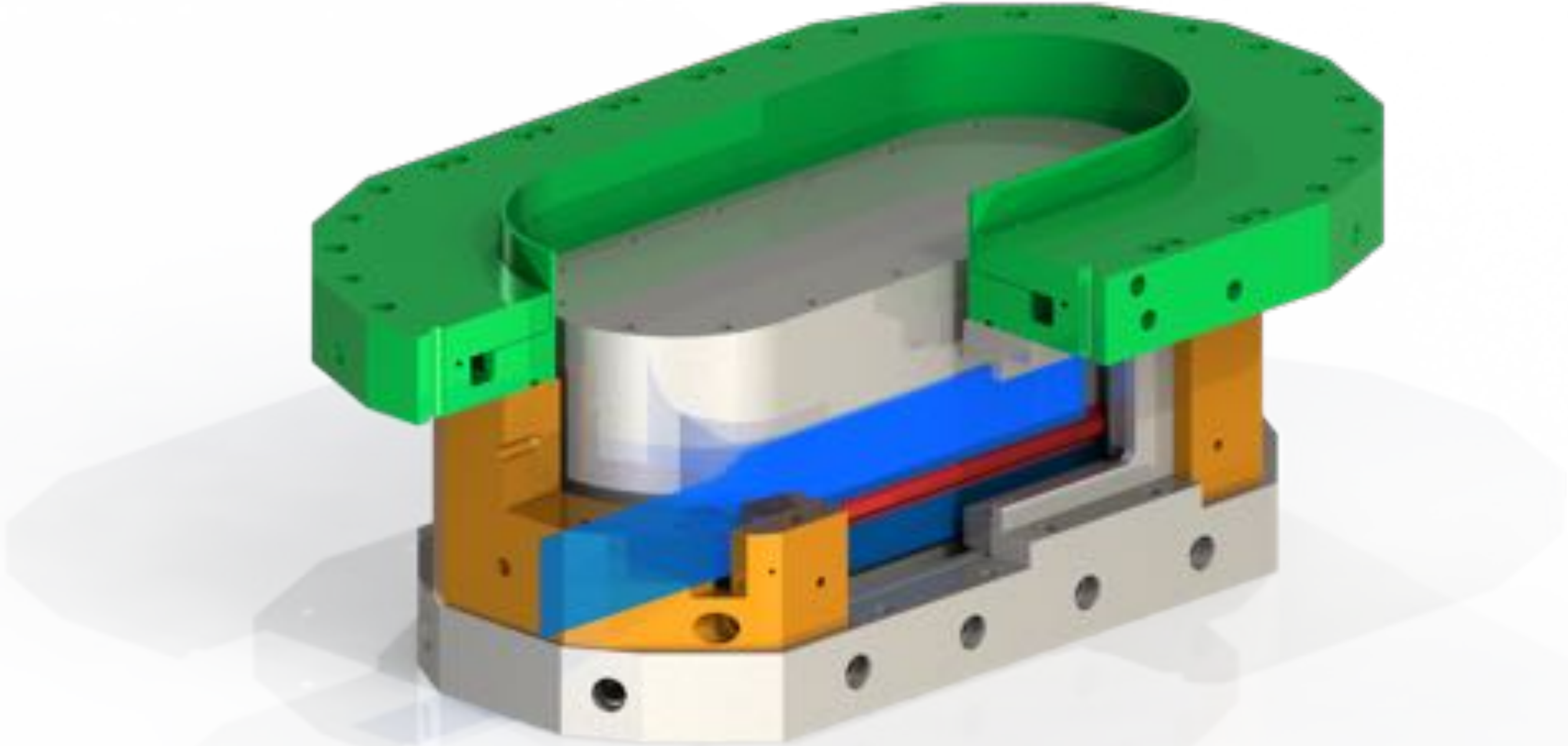

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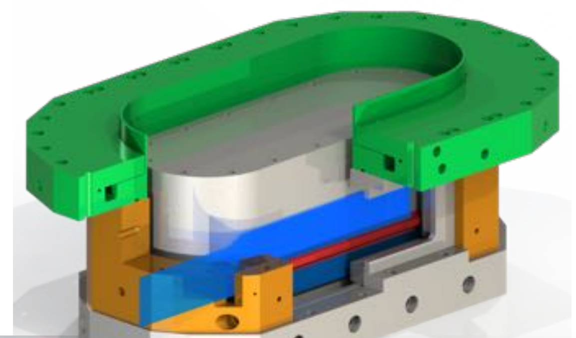
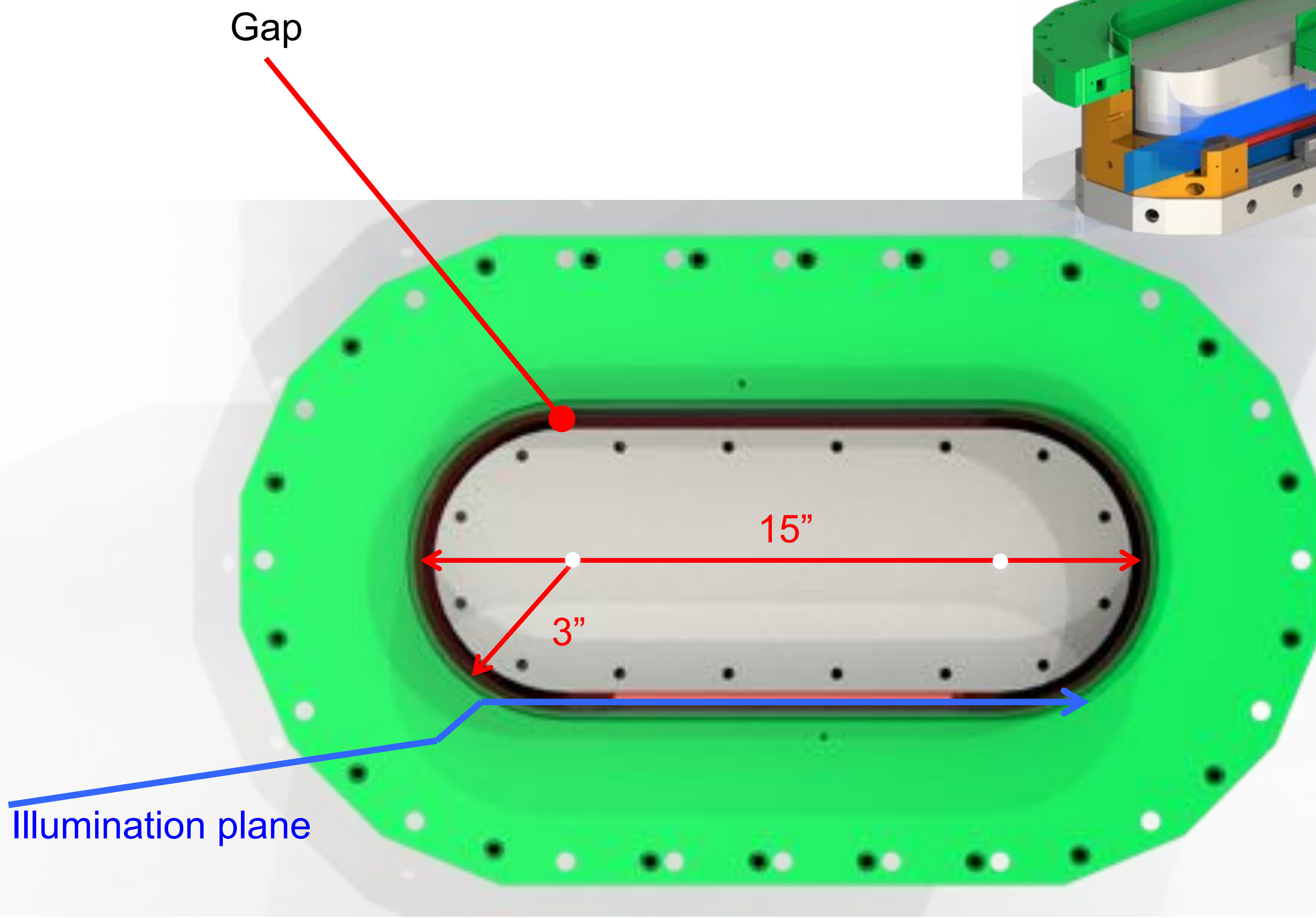
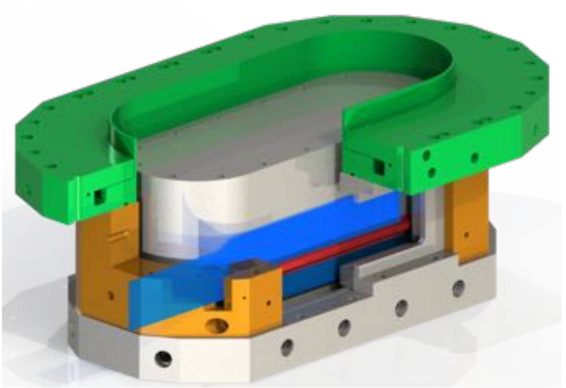


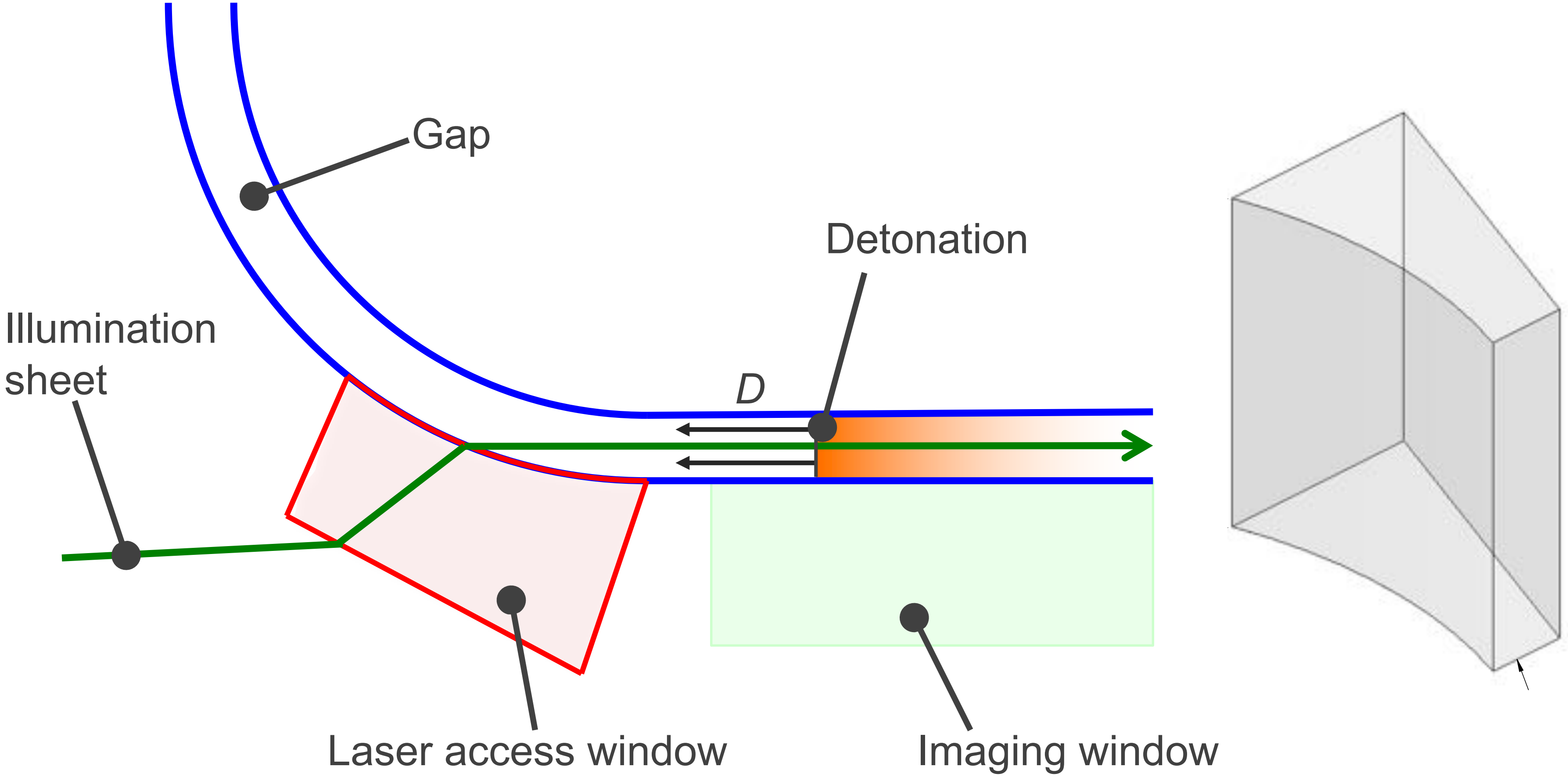


Proposed Hybrid RDE (Race Track RDE, or RT-RDE)

Our design:

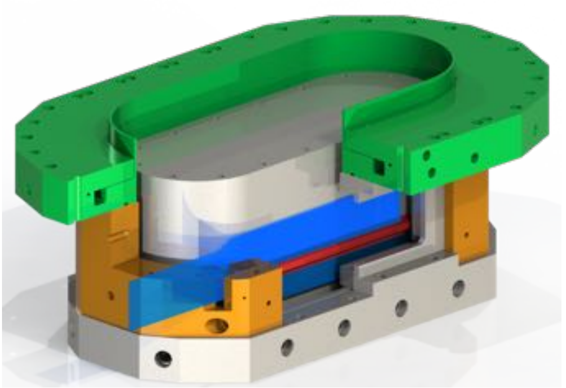
- Resolves optical access limitations of round RDE
- But optical access through curved wall is required
- We have designed an optical arrangement to access the detonation chamber through curved wall





Proposed Hybrid RDE (Race Track RDE, or RT-RDE)

Our design:



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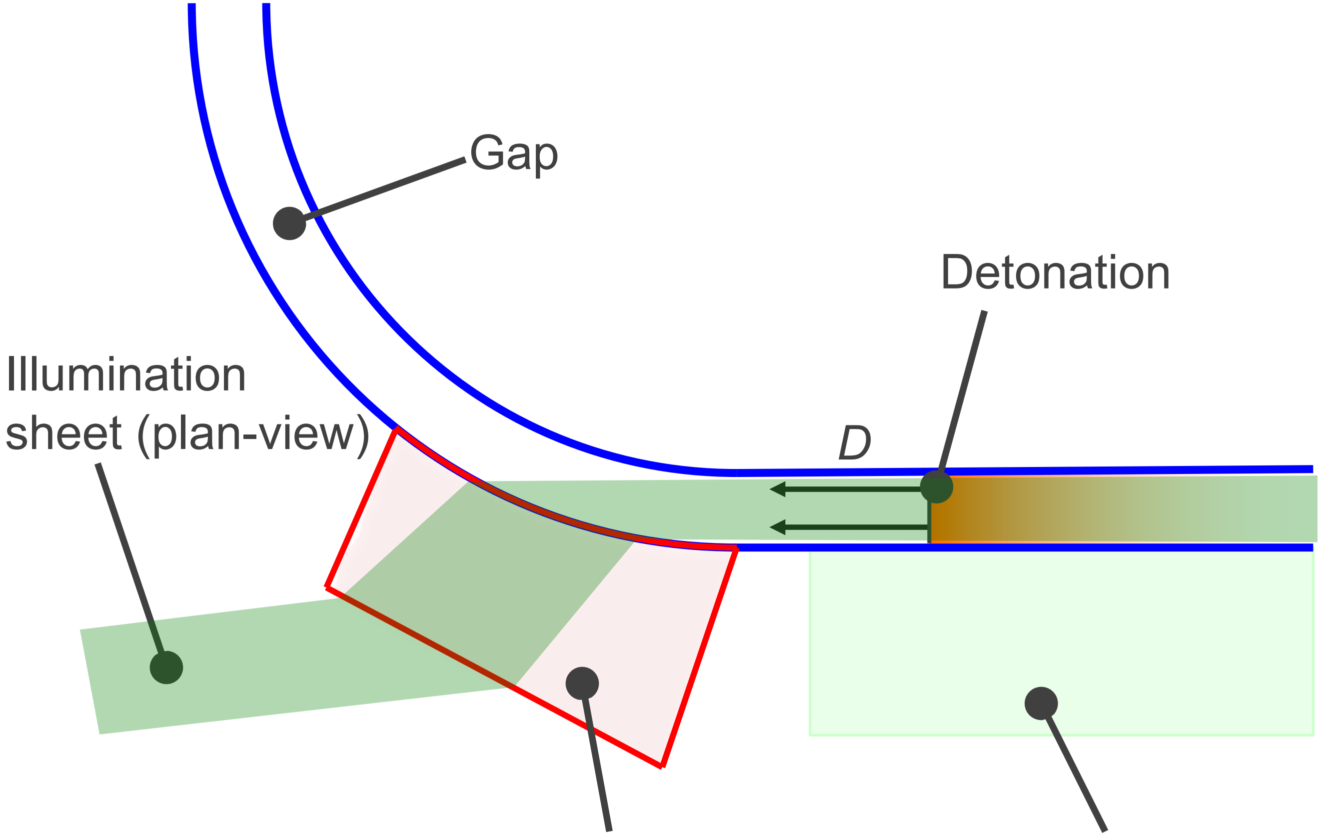
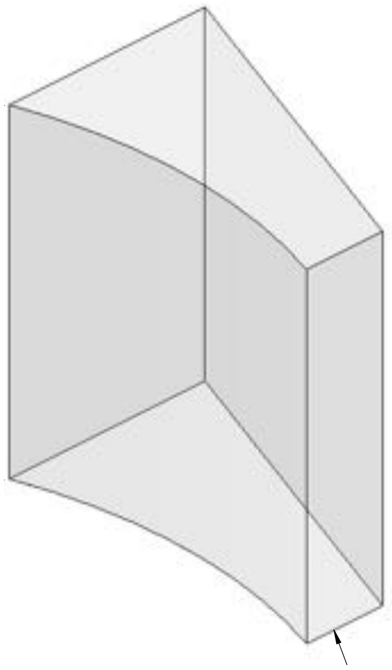




Next steps for experimental program

- Detailed studies of shock-induced mixing in single and multiple injector configurations
  - All systems operational
  - Complete mixing measurements on parametric study
- RDE
  - Complete integration of RDE and testing
  - Investigation of performance of different injectors
  - Inform future work on RT-RDE
- RT-RDE
  - Verify optical access design (prototype window should be delivered this month)
  - Fabrication and instrumentation (design is complete, shop selected)
  - Investigate detonation structure and the link between unmixedness, detonation structure and pressure gain
    - Speciation distribution
    - Detonation speed and height, pressure time history
    - Transition and stabilization to deflagration mechanisms

Outline

- Introduction to the problem and general approach
- Experimental activities
- Computational activities

Computational Study of Non-idealities in RDEs

Venkat Raman
University of Michigan

Outline of Simulation Results

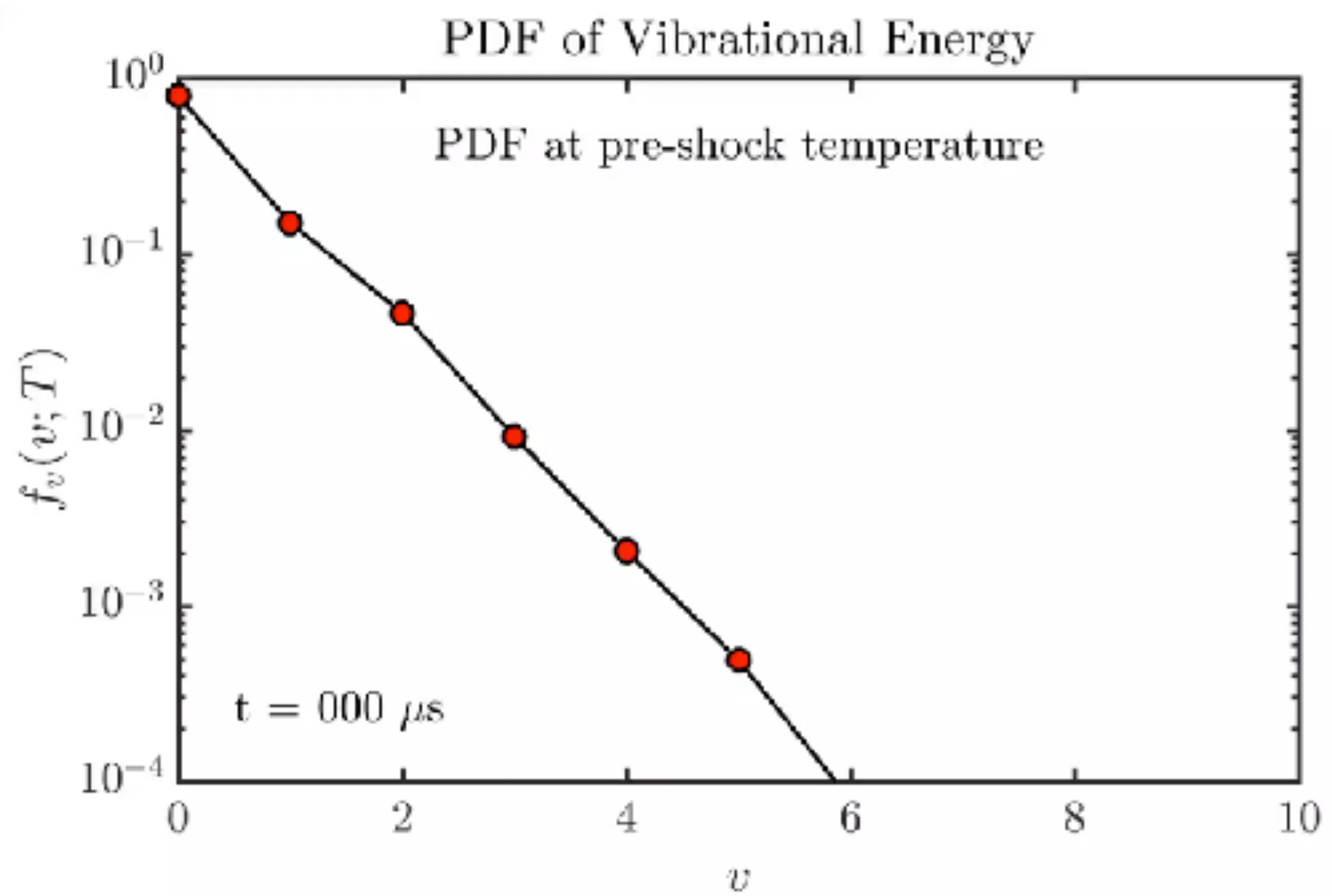
- **Effect of nonequilibrium on detonation cell size**
- **Effect of injector mixing on detonation propagation**
  - ➡ Blast wave/detonation comparison
  - ➡ Multi-injector DNS
  - ➡ Detonation structure analysis

Thermal Nonequilibrium Modeling Considerations

Thermal equilibrium is not preserved through shocks,
resulting in underpopulated vibrational states

- Relaxation depends on species and collision timescales
- Relevant if relaxation is comparable to reacting and mixing scales, i.e.,

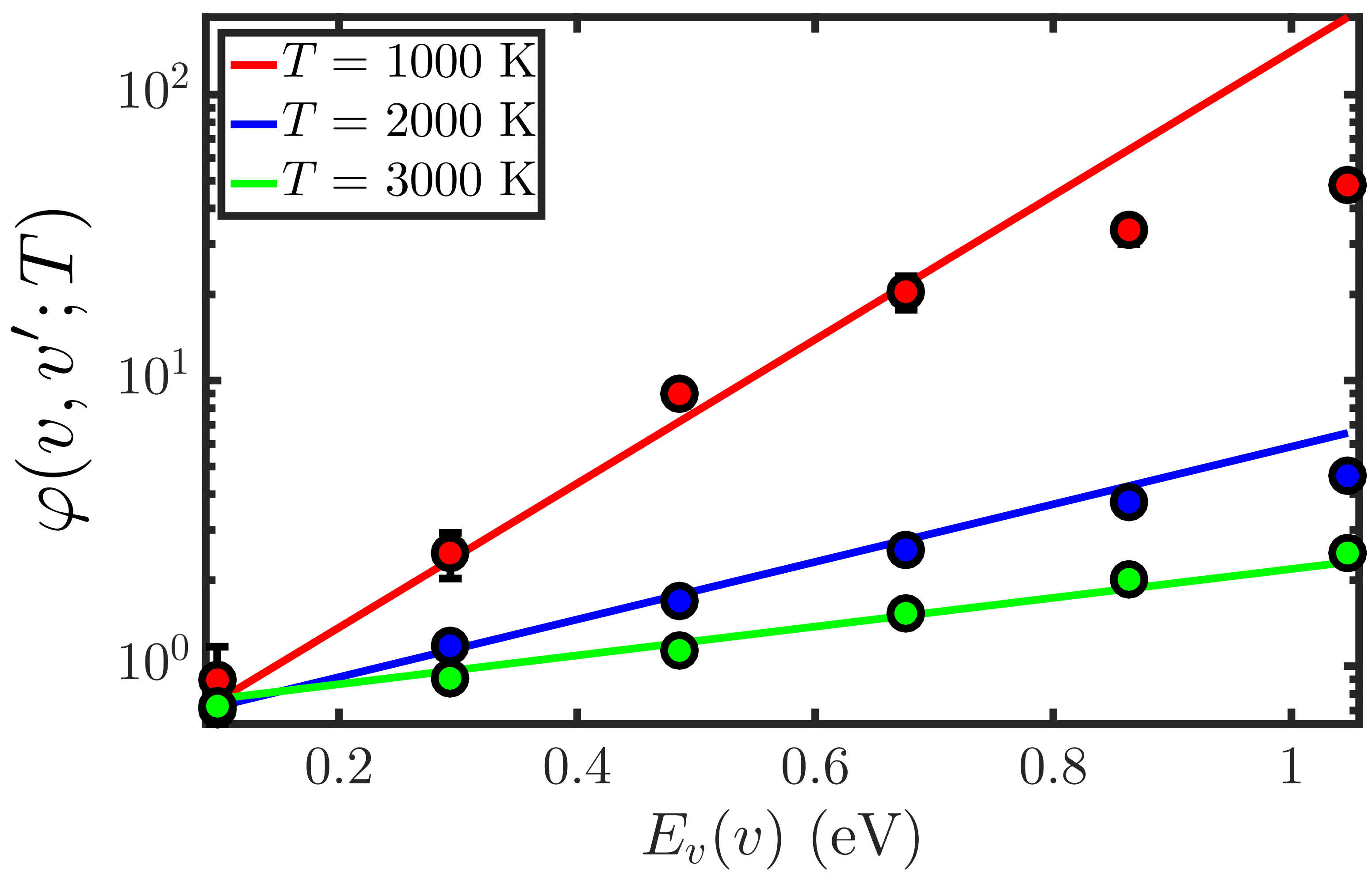
$$\tau_{relax} \approx \min(\tau_{react}, \tau_{flow})$$

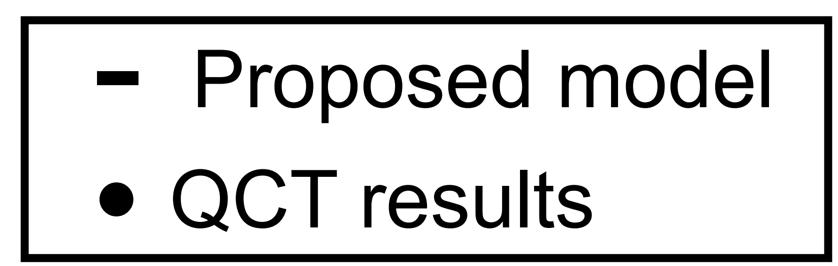


Vibrational Nonequilibrium: Ab-initio Derived Rates

- **QCT-based state-specific reaction rates used to calibrate model**
  - ➡ Model matches QCT results at high temperatures
  - ➡ Nonlinear/higher-order model required at lower temperatures

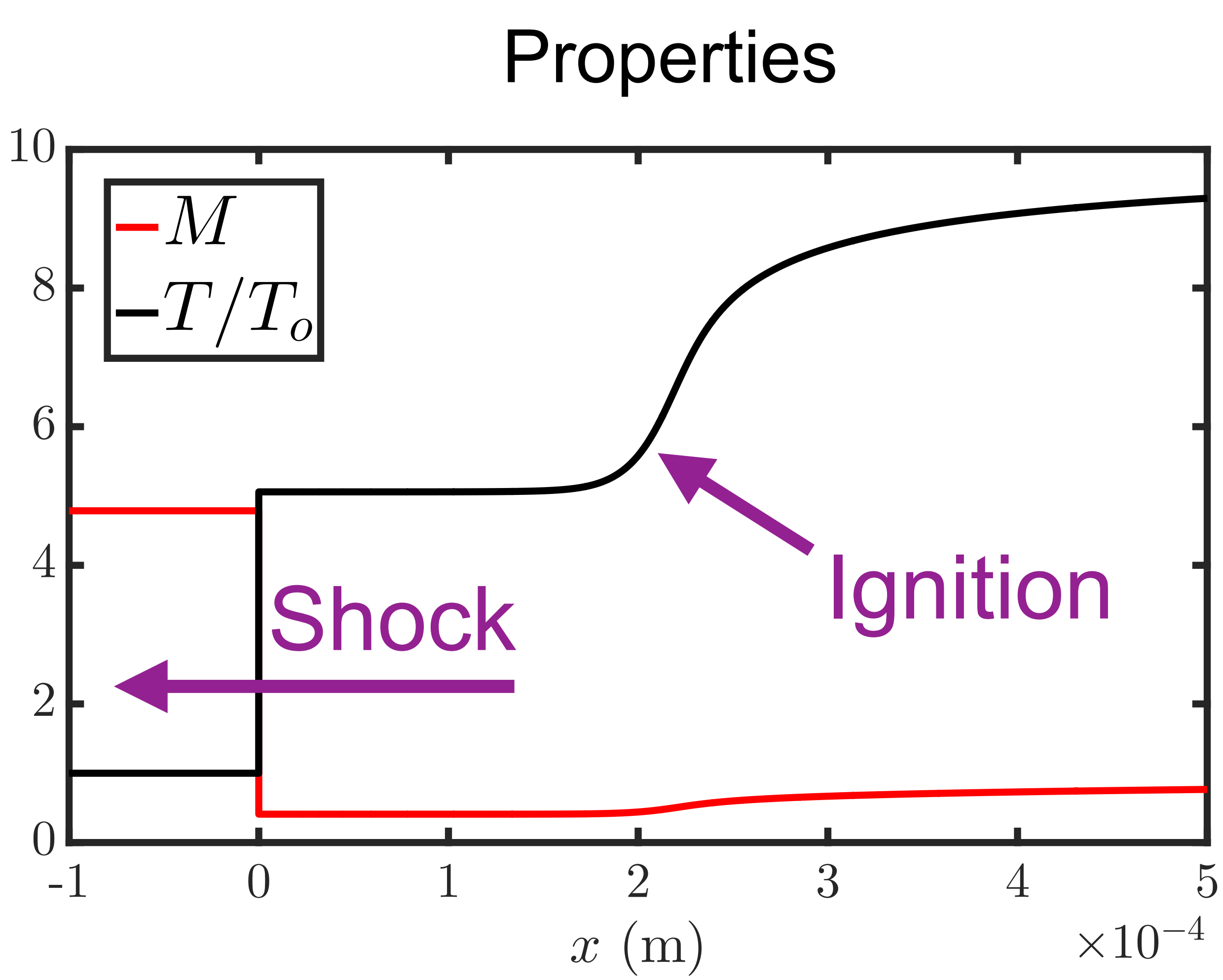
$$H + O_2(v) \longrightarrow O + OH$$

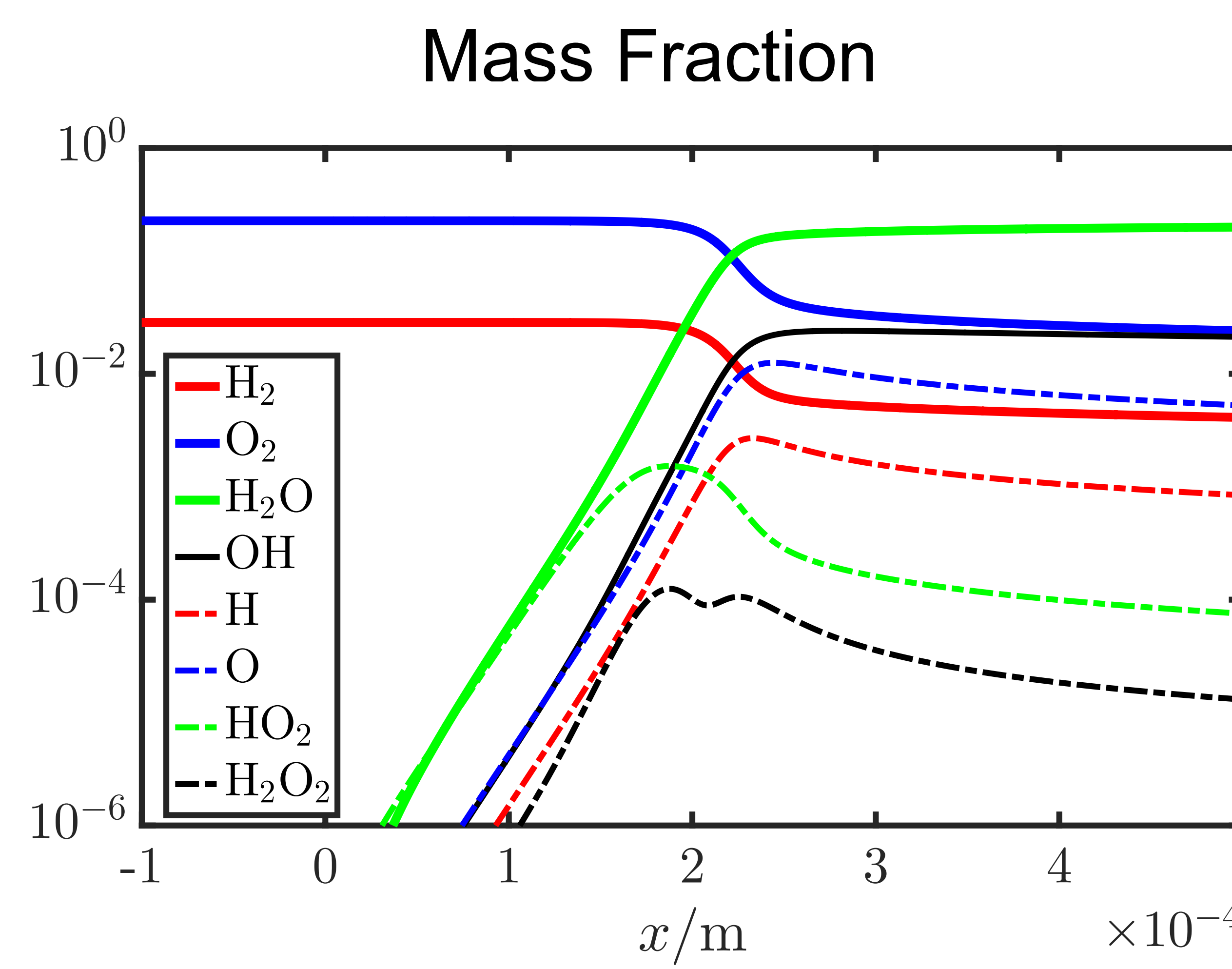




Detonation Wave Simulation: Equilibrium Case

- **Baseline solution simulated assuming thermal equilibrium**
  - ➡ Stoichiometric hydrogen-air mixture initially at 300 K and 1 atm
  - ➡ Ignition length near 2.1x10^{-4} m from the shock front (≈1x10^{-4} s)
  - ➡ Temperatures pre-shock, post-shock, and post-combustion are 300, 1510, and 2920 K





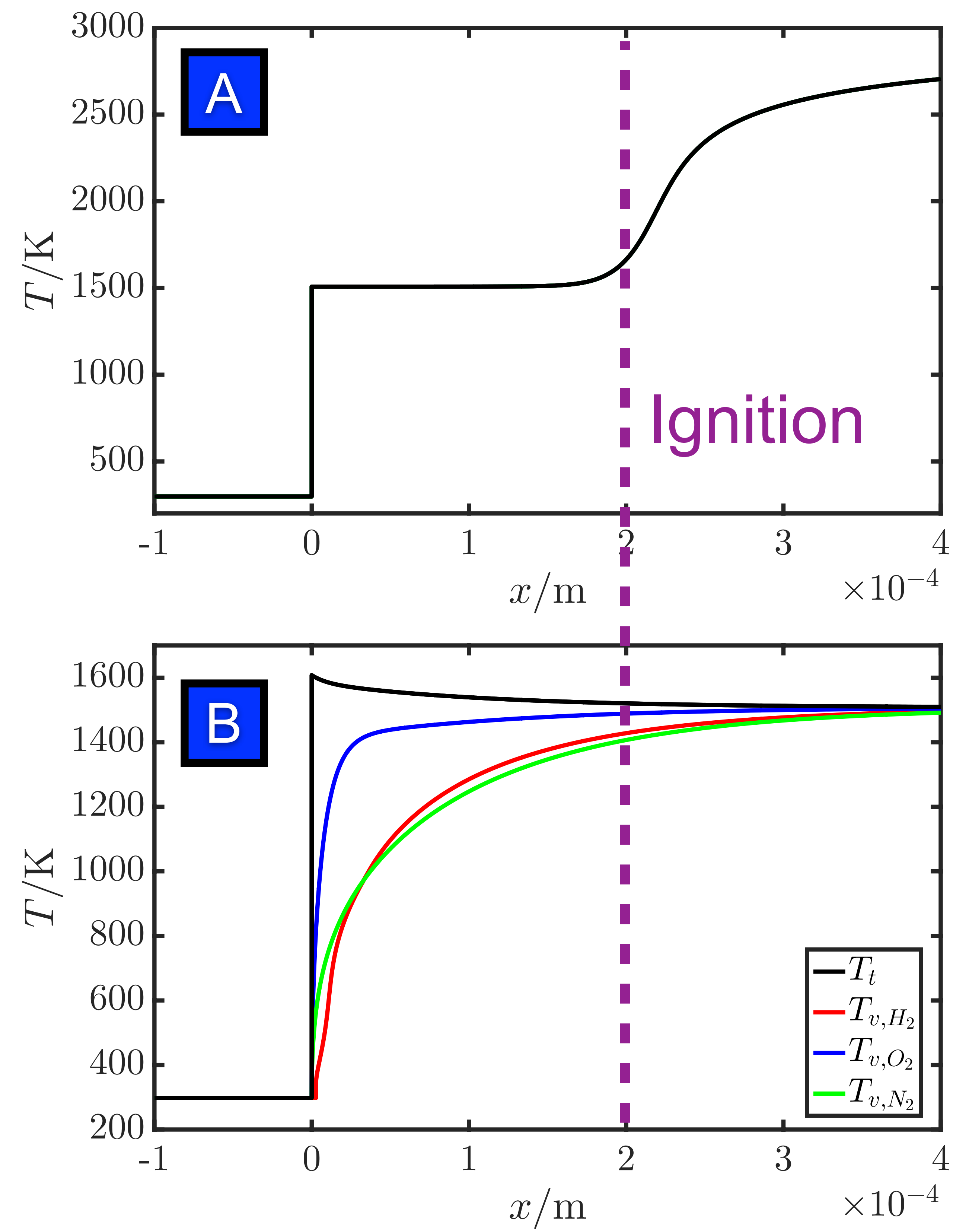
Detonation Wave Simulation: Relaxation Scales

- **Recall the nonequilibrium relaxation factor:**

$$\frac{\tau_{relax}}{\min(\tau_{reac}, \tau_{flow})}$$

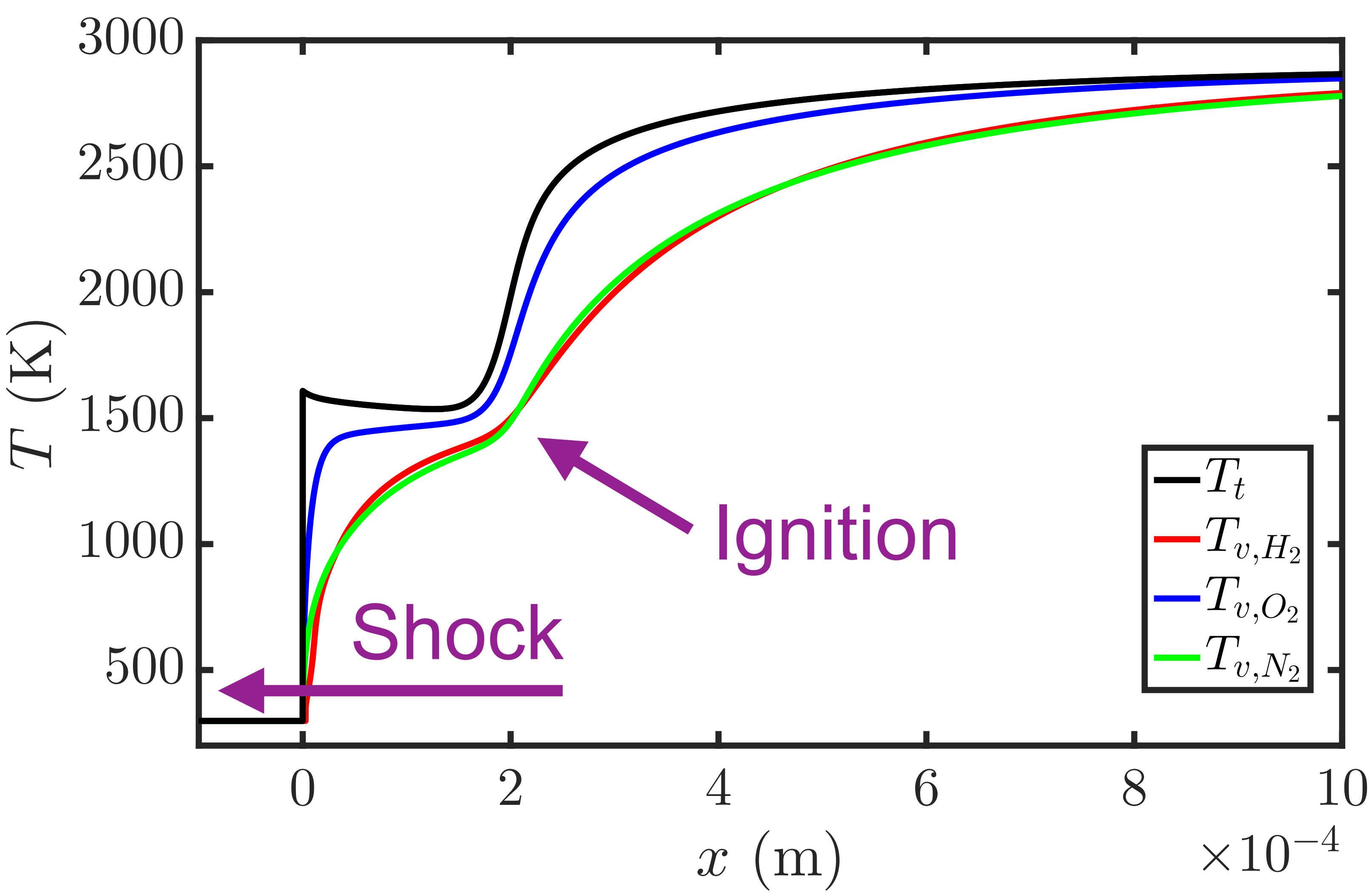
- **Consider two simulations:**
  - ➡ A Reactive simulation with thermal equilibrium
  - ➡ B Inert simulation with <u>vibrational nonequilibrium</u>
    - O_2 relaxes to a quasi-steady state within $2\text{x}10^{-5}$ m
    - H2 and N2 relax more slowly

$$\frac{\tau_{relax}}{\min(\tau_{reac}, \tau_{flow})} \approx \mathcal{O}(1)$$



Detonation Wave Simulation: Nonequilibrium Case

Nonequilibrium simulation demonstrates necessity for species-specific vibrational temperatures

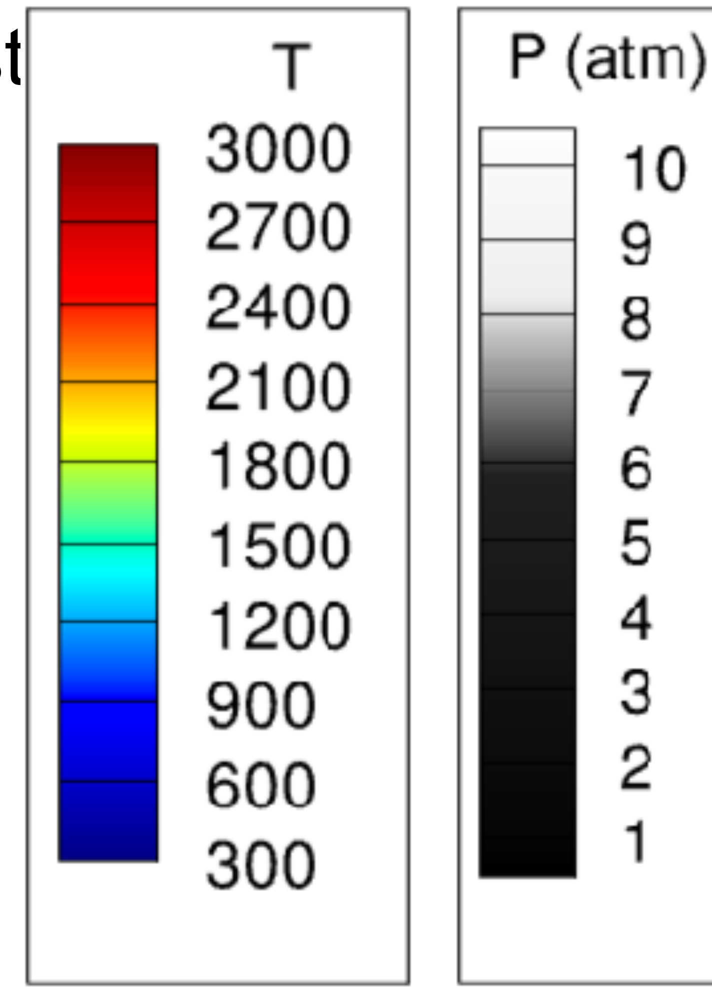


Temperature of detonation wave with vibrational nonequilibrium

- O_2 rapidly approaches quasi-steady-state via T-V exchange
- Induction length is comparable to equilibrium case

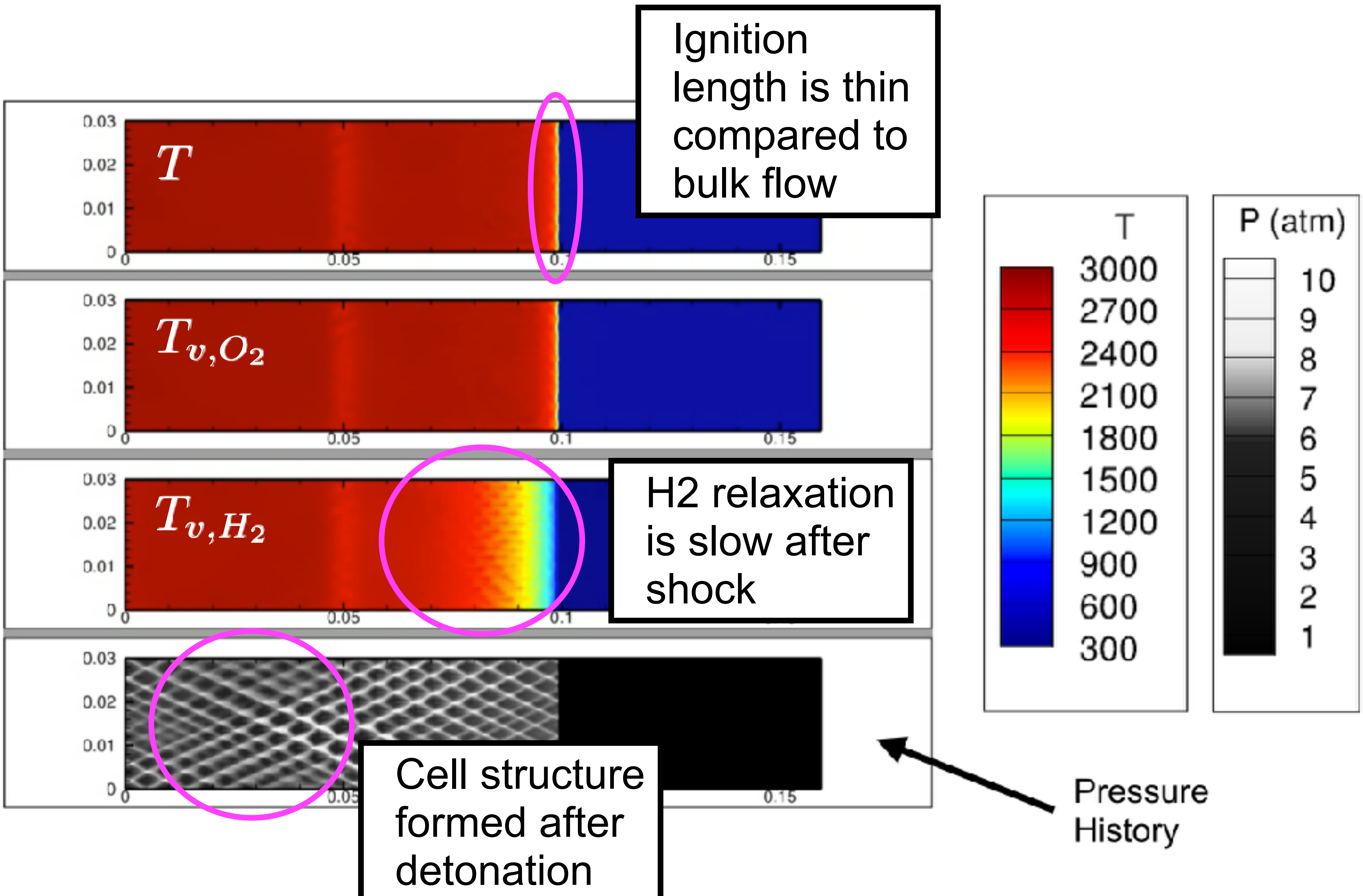
2D Detonation Wave Simulation

- **2D detonation wave simulated to assess vibrational nonequilibrium effects on detonation cell-pattern regularity**
  - ➡ Initial conditions based on the 1D simulation at equilibrium conditions, then simulated along channel until st
  - ➡ Simulated on 5000 cores over 10 hours



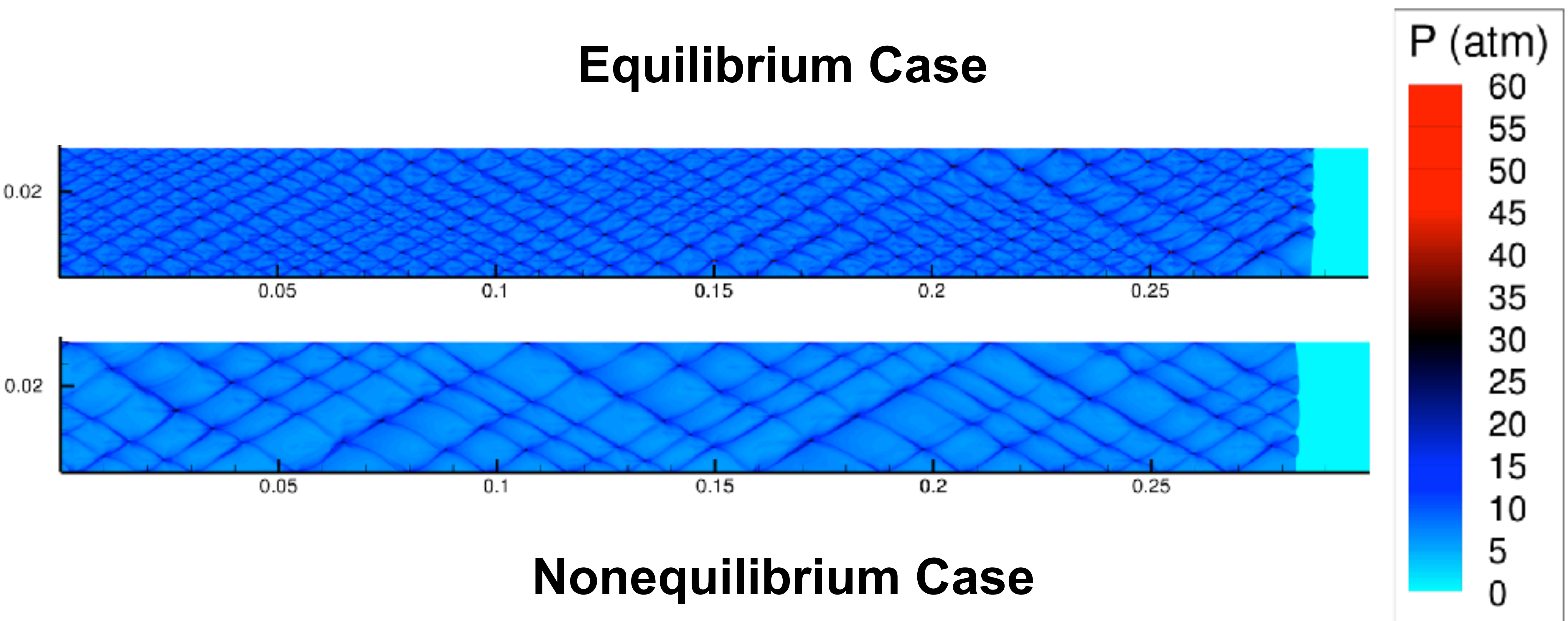
Pressure History

2D Detonation Wave Simulation



2D Detonation Wave Simulation

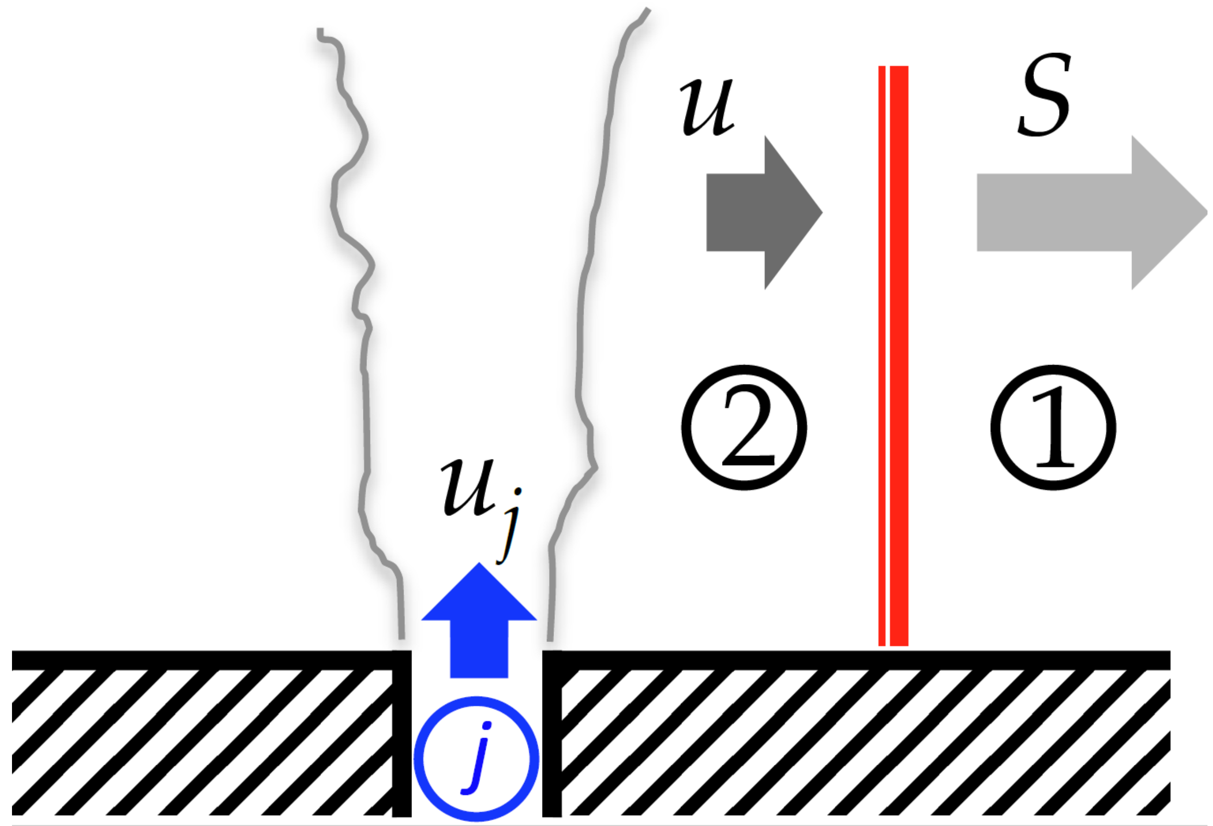
- **The pressure history shows that modeling vibrational nonequilibrium significantly modifies detonation cell size**
  - ➡ Delayed relaxation of H_2 plays a critical role in this process
  - ➡ In both cases, detonation cells are unstable



Blast Wave/Detonation Analogy

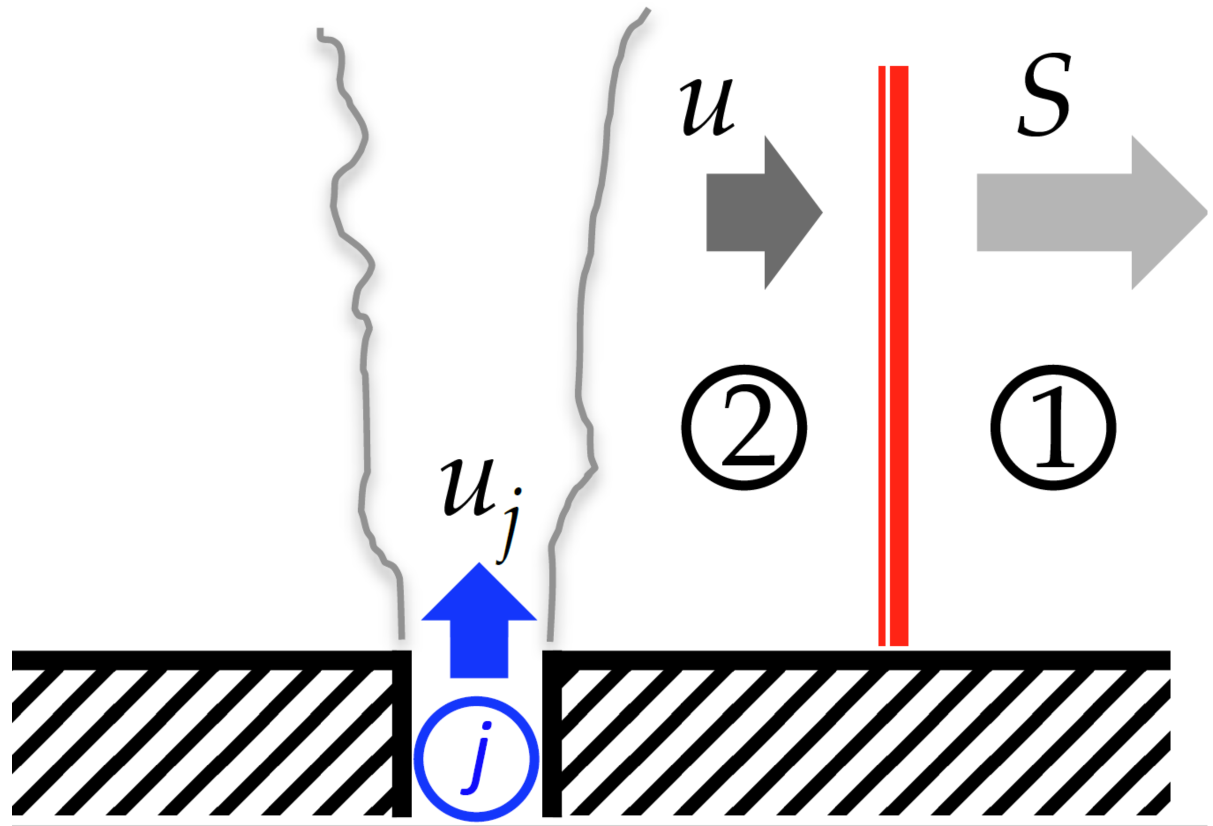
- **Can blast waves with appropriate conditions used to understand mixing in detonations?**
  - ➡ Easier experiment to do
  - ➡ Access to better laser diagnostic tools
- **Numerical study**
  - ➡ Conduct blast wave and detonation studies
  - ➡ Identify mixing parameters

Blast wave conditions



	1	2	jet
P (Pa)	66700	226880	66700
T (K)	298	486.42	298
rho (kg/m3)	8.4977E-01	1.77	5.4274-02
U (m/s)	0	288.8	418
comp (H2-O2-Ar mole)	2-1-7	2-1-7	1-0-0

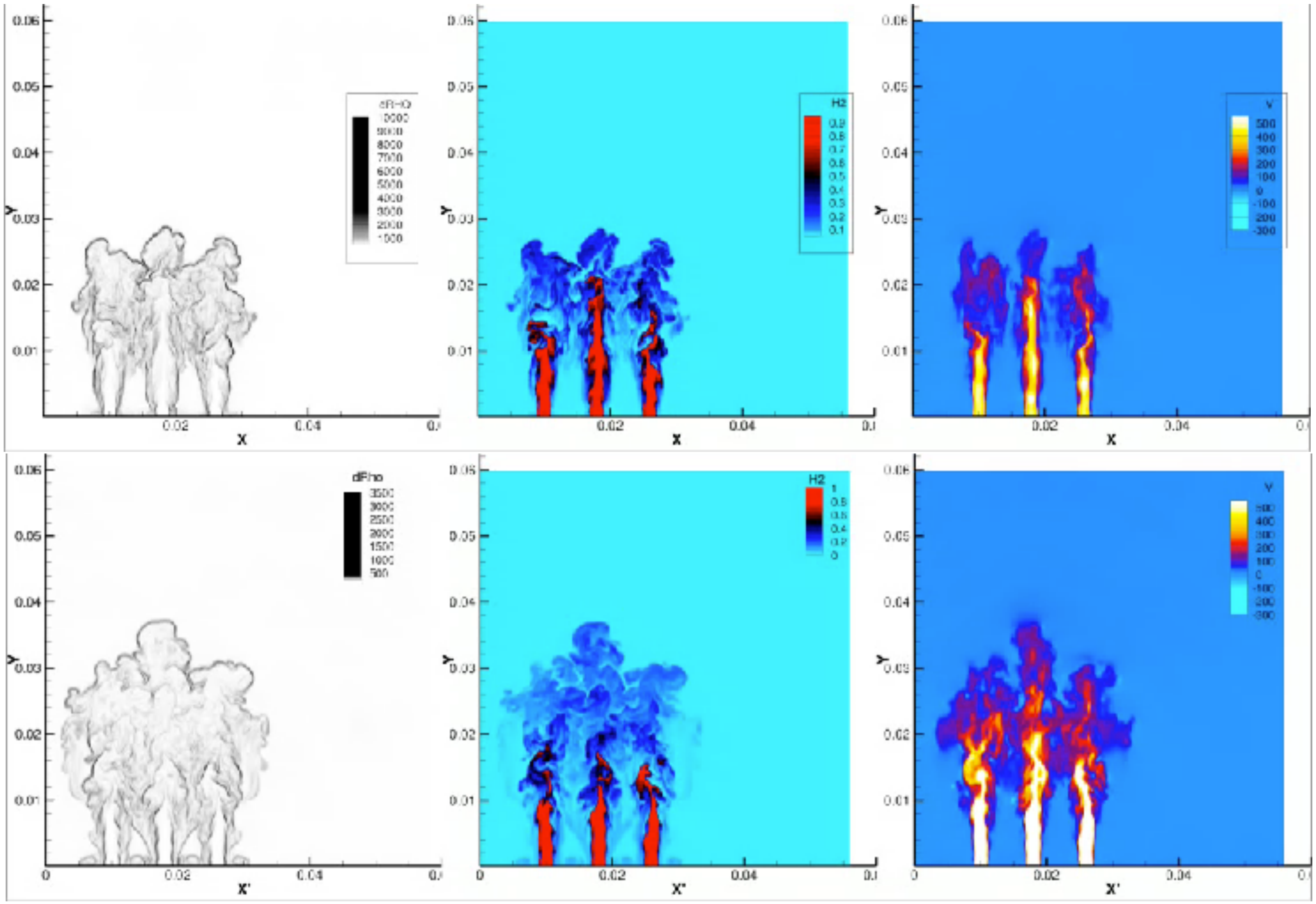
Detonation conditions



	1	2	jet
P (Pa)	6670	125000	6670
T (K)	298	2850	298
rho (kg/m3)	8.4977E-02	0.177	5.4274-03
U (m/s)	0	830	526.5
comp (H2-O2-Ar mole)	2-1-7	burnt products	1-0-0

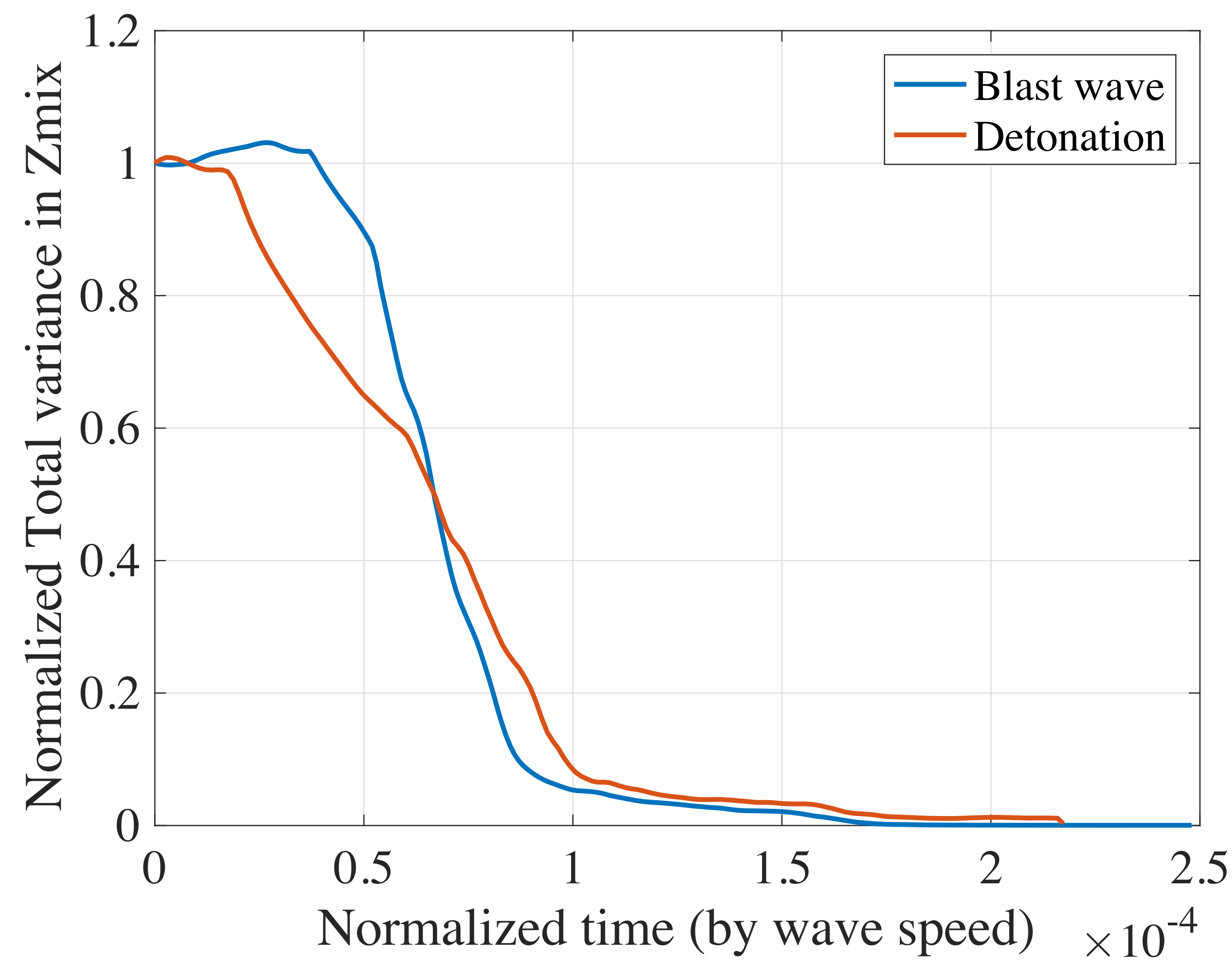
3 Jet mixing comparison : blast wave/detonation

- Premixed H_2-O_2-Ar at 298K, 6670Pa and pure H_2 injectors
- Conserved properties : ρ_{jet}/ρ_2 and u_{jet}/u_2



Preliminary Mixing Metrics

- **Scalar variance seems to decay in a similar manner**
  - ➡ Density change the primary driver for enhanced mixing
- **Post-wave mixing is driven only by decaying turbulence**
  - ➡ Similar for both blast waves and detonations

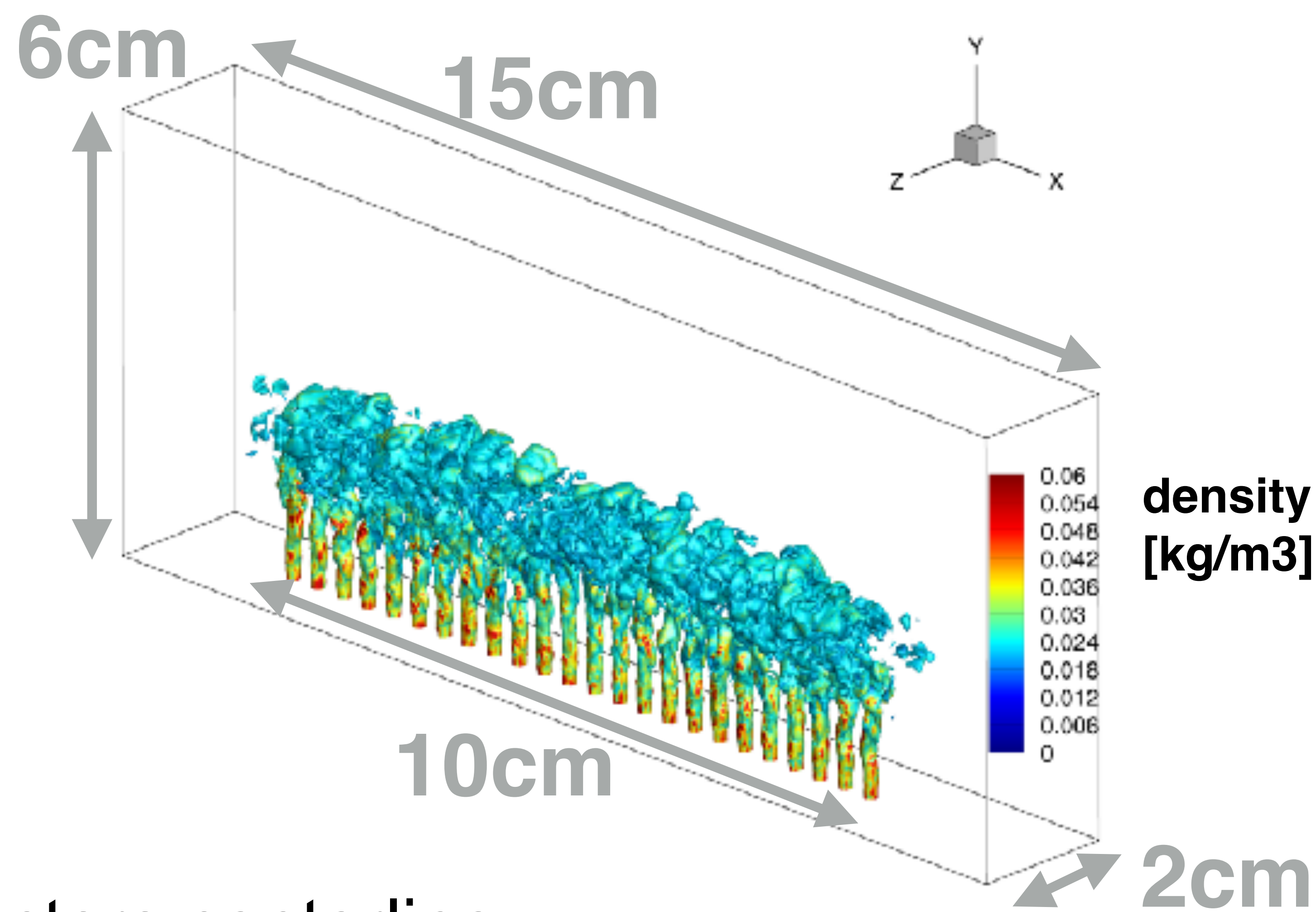


Multi-Injector Configurations

- **RDEs employ discrete injectors**
  - ➡ Premixed or non-premixed
- **In non-premixed injectors**
  - ➡ Level of mixing can control detonation propagation
- **How does injector mixing affect detonations?**
  - ➡ Influence of small-scale mixing
  - ➡ Large scale impact
  - ➡ Distance between injectors
- **Goal: Develop a canonical linear RDE setup for studying mixing effects**

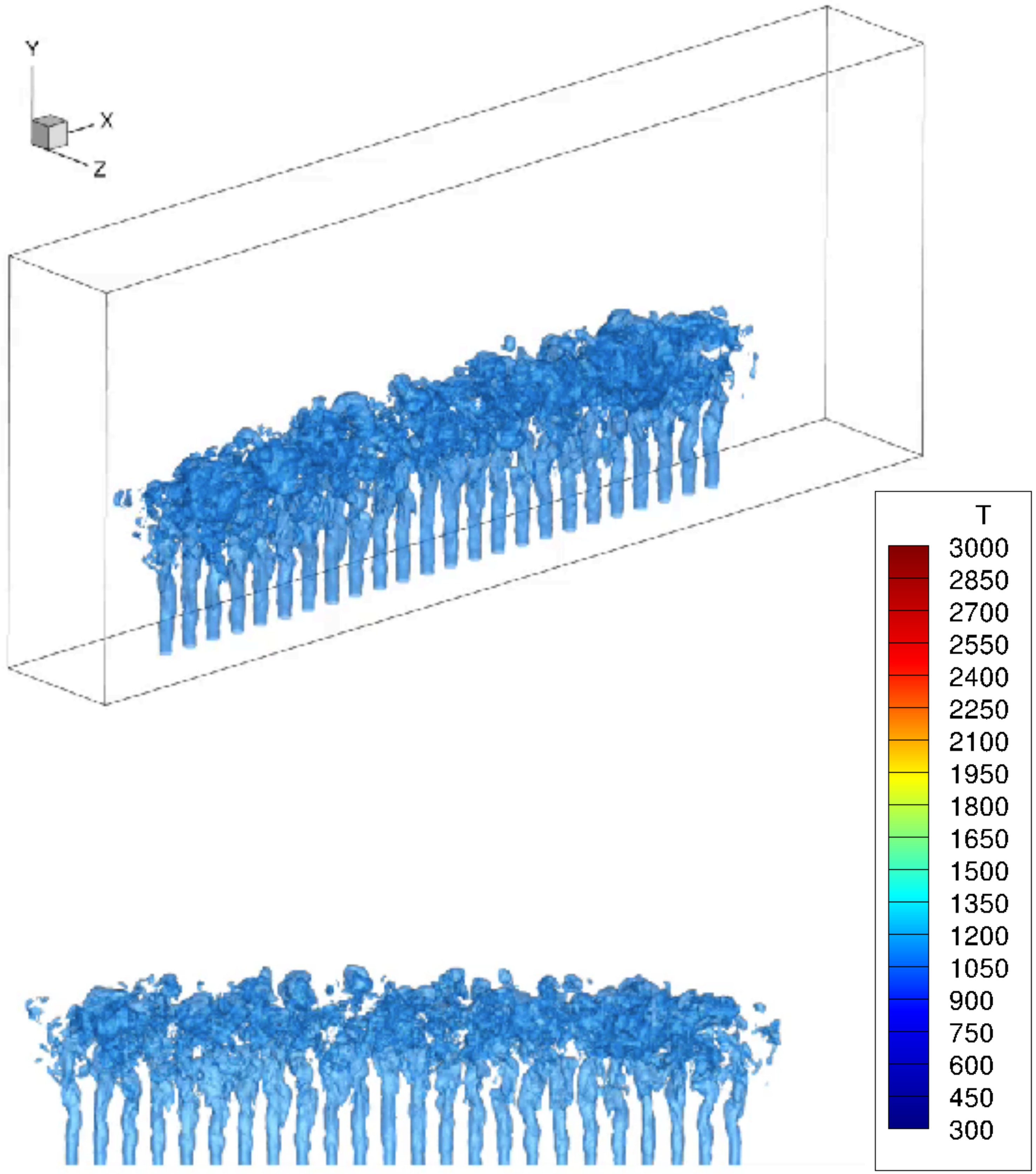
Numerical Study of Multi-injector Configurations

- **For all simulations**
  - ➡ Injection zone Lj = 10cm
  - ➡ Fuel mass flow rate Fj
- **Variables**
  - ➡ Nj = number of injectors
  - ➡ Dj = injectors diameter
  - ➡ dXj = distance between injectors centerline
  - ➡ Mj = injector exit Mach number



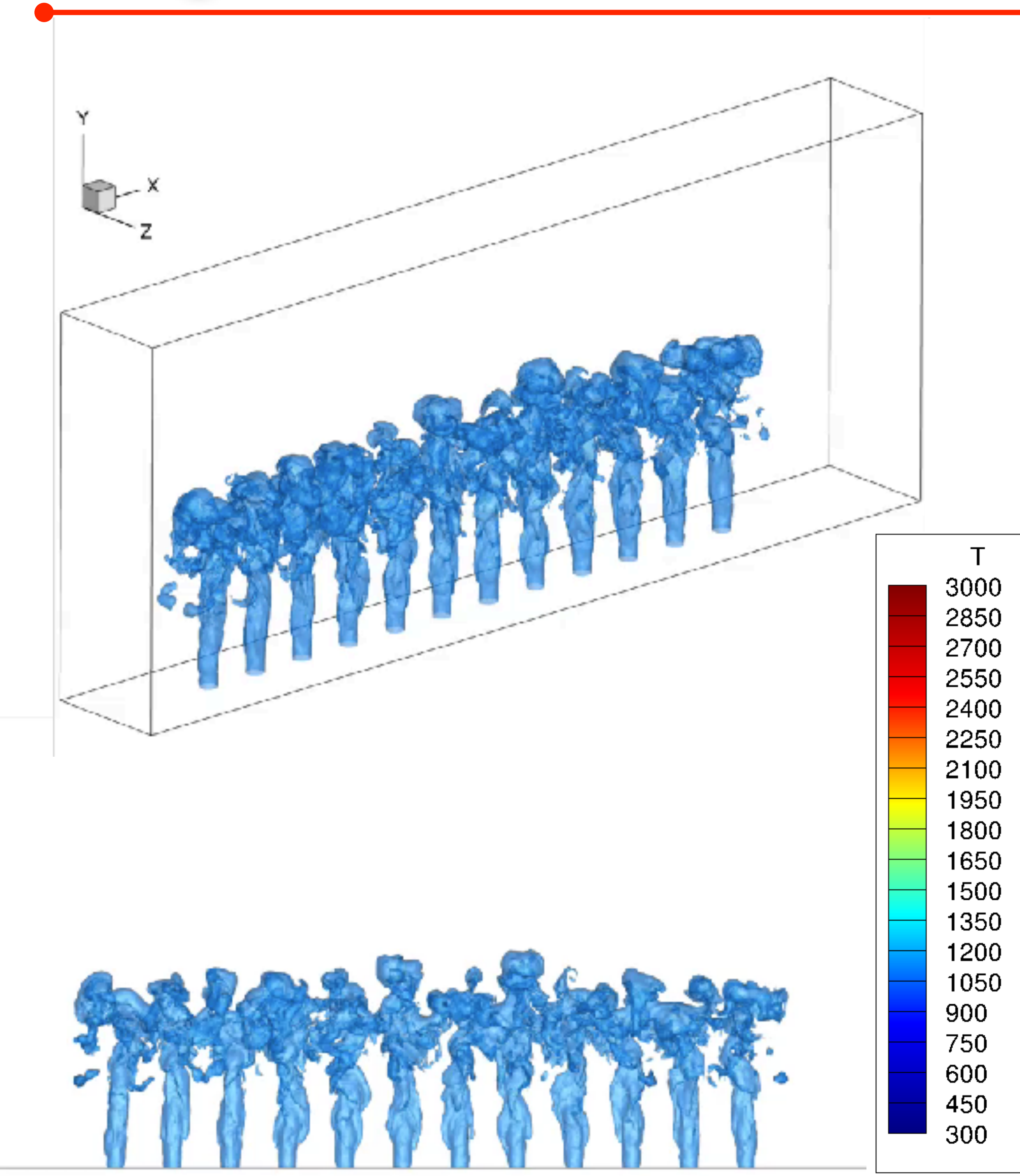
Configuration	Nj	Dj [mm]	dXj [Dj]	Mj
S	24	1.63	2.67	0.83
M	16	2.00	3.33	0.83
L	12	2.55	3.56	0.68
XL	8	3.55	4.03	0.53

Configuration S



- **Isocontours of**
  - ➡ H2 = 0.1
  - ➡ T = 800K (black)
  - ➡ log(|q|) = 9.5
- **Colored by temperature**

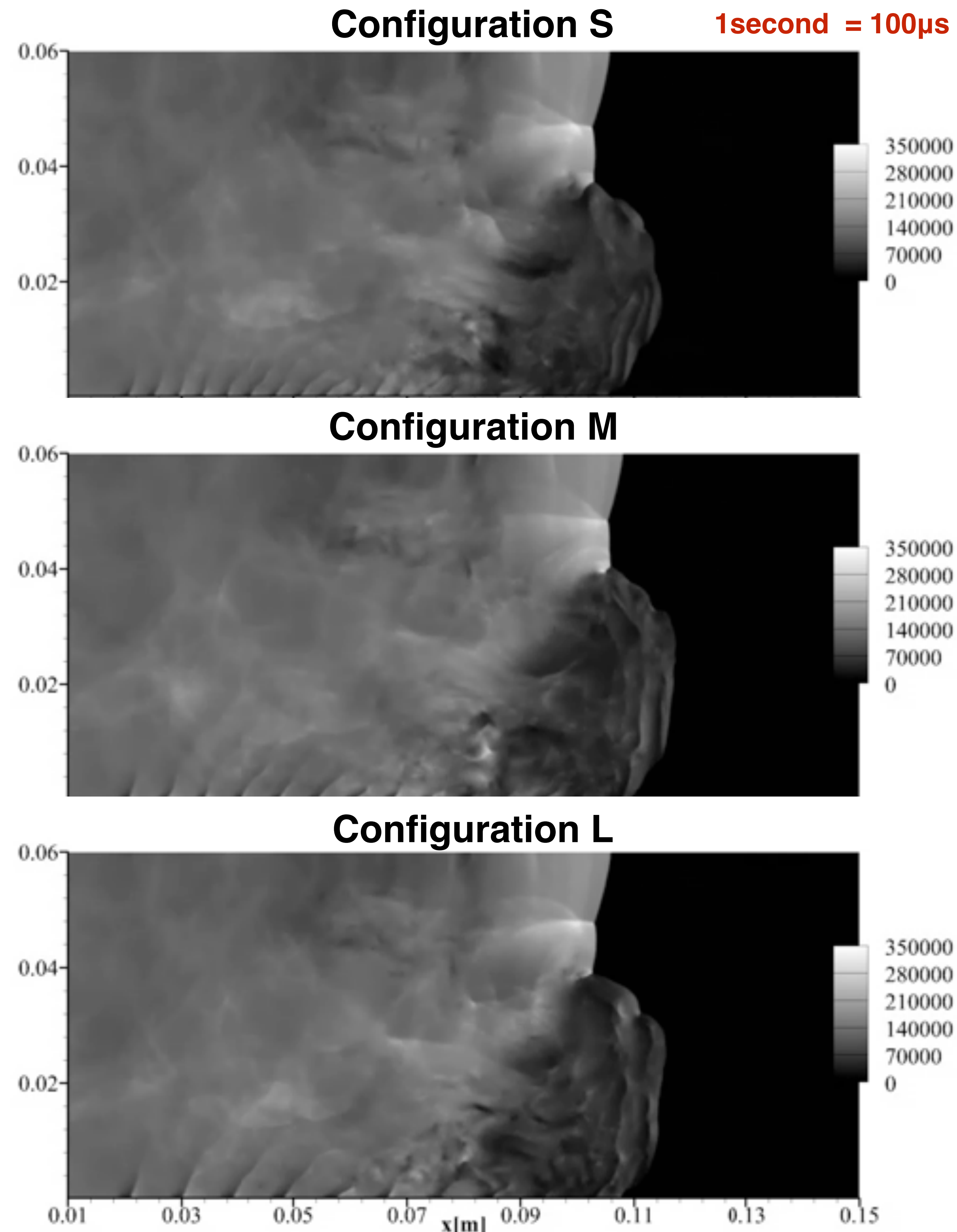
Configuration L



- **Isocontours of**
  - ➡ H_2 mass fraction of 0.1
  - ➡ Temp. of 800K (black)
  - ➡ log(|q|) = 9.5
    - Q-criterion
- **Colored by temperature**

Post-detonation Explosions

- **Shock wave interactions**
  - ➡ Regular high-pressure spots
  - ➡ Creates regular post-detonation explosions
- **Frequency is independent of the injector configuration**
  - ➡ Independent of ambient conditions
    - [To be discussed next]



Effect of Ambient Conditions

- **Simulations so far**
  - ➡ Consider first passage of detonation wave
  - ➡ Cold oxidizer as ambient condition
- **RDE conditions**
  - ➡ Some pre-burnt mixture from prior detonations will be present
- **How does ambient composition affect detonations?**
  - ➡ Can there be pre-ignition and loss of efficiency?

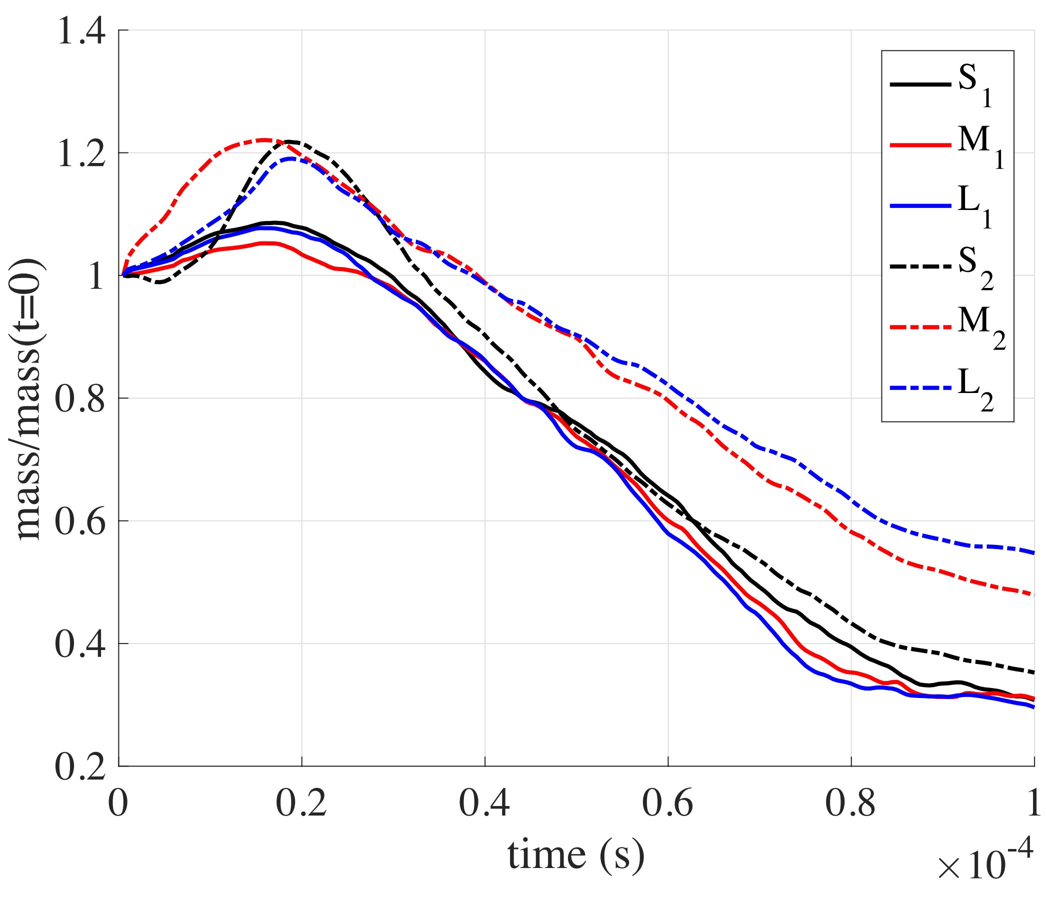
Variation of downstream mixture

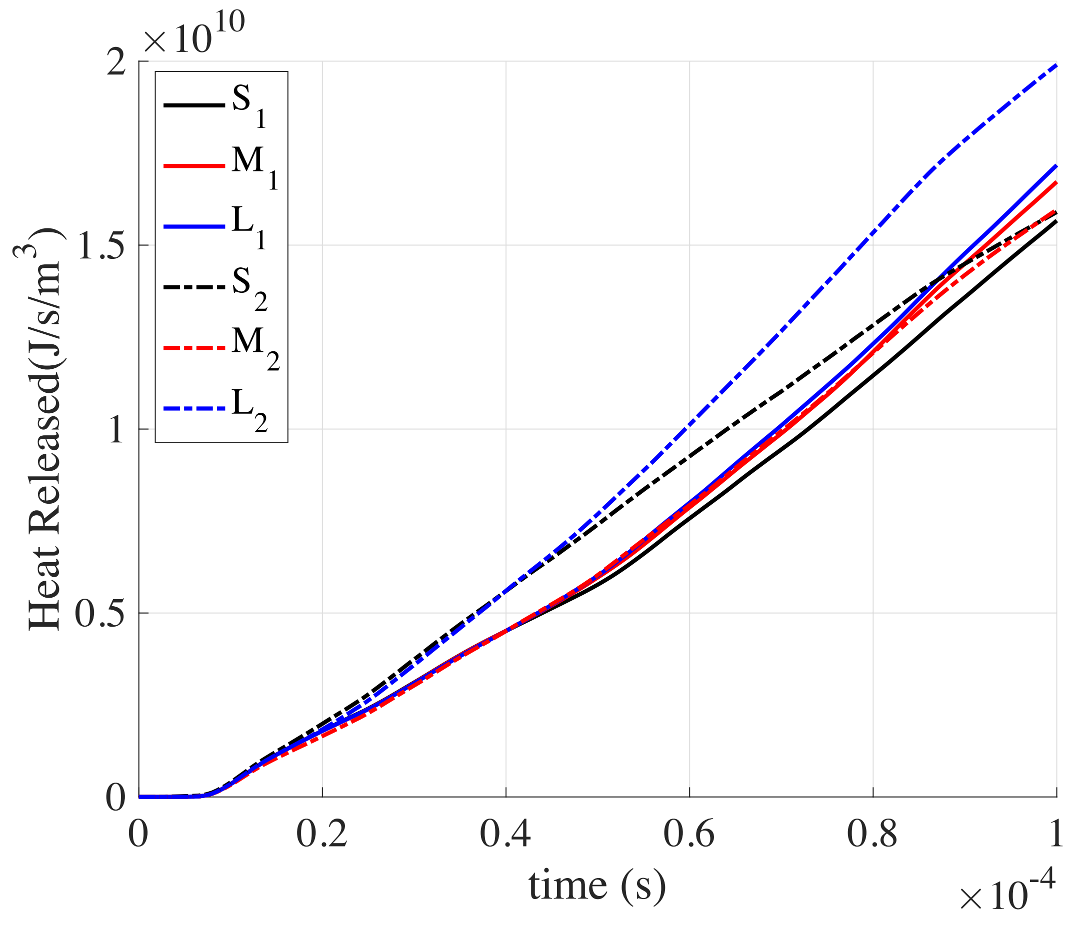
- **Case I represents the first passage of the detonation**
  - ➡ Clean Ar-O2-H2 mixture
  - ➡ Low temperature and pressure
- **Case II represents a second passage of the detonation**
  - ➡ Partially burnt Ar-H2O-O2-H2 mixture
  - ➡ Higher temperature and pressure

Configuration	$P_{jet}/P_{ambient}$ (Pa)	T_{jet} (K)	$T_{ambient}$	Ambient composition
Case I	6670	298	298	O_2 / Ar (1/7)
Case II	33350	298	2200	H_2O / O_2 / Ar (1/2/14)

Integrated Fuel Consumption and Heat Release

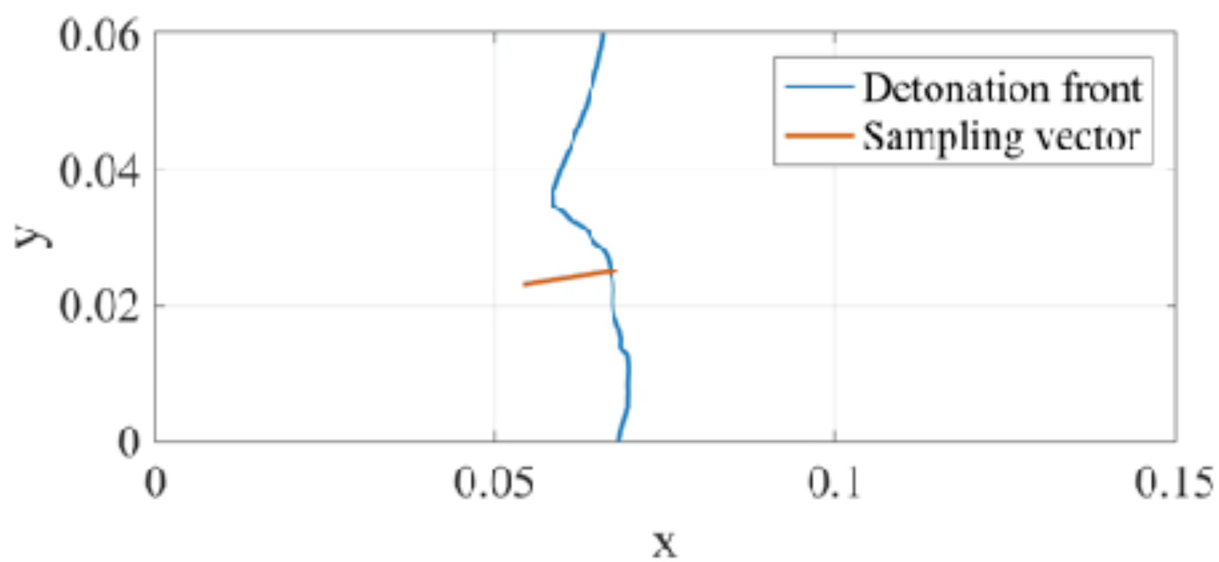
- **Initial indication is that ambient conditions do not significantly affect detonation process**
  - ➡ Mass consumption rates are unaltered
  - ➡ Additional conditional statistics being analyzed currently



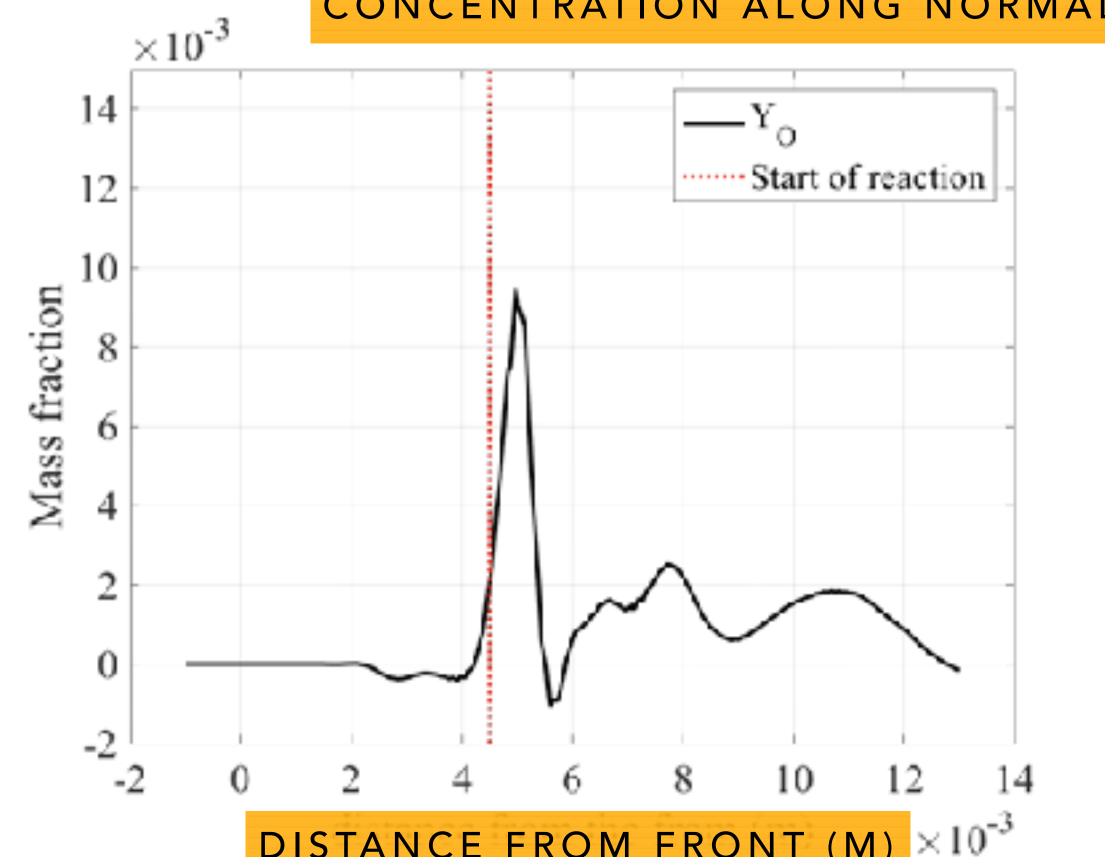


Front-tracking and Induction Length

DETONATION PROFILE AND NORMAL VECTOR



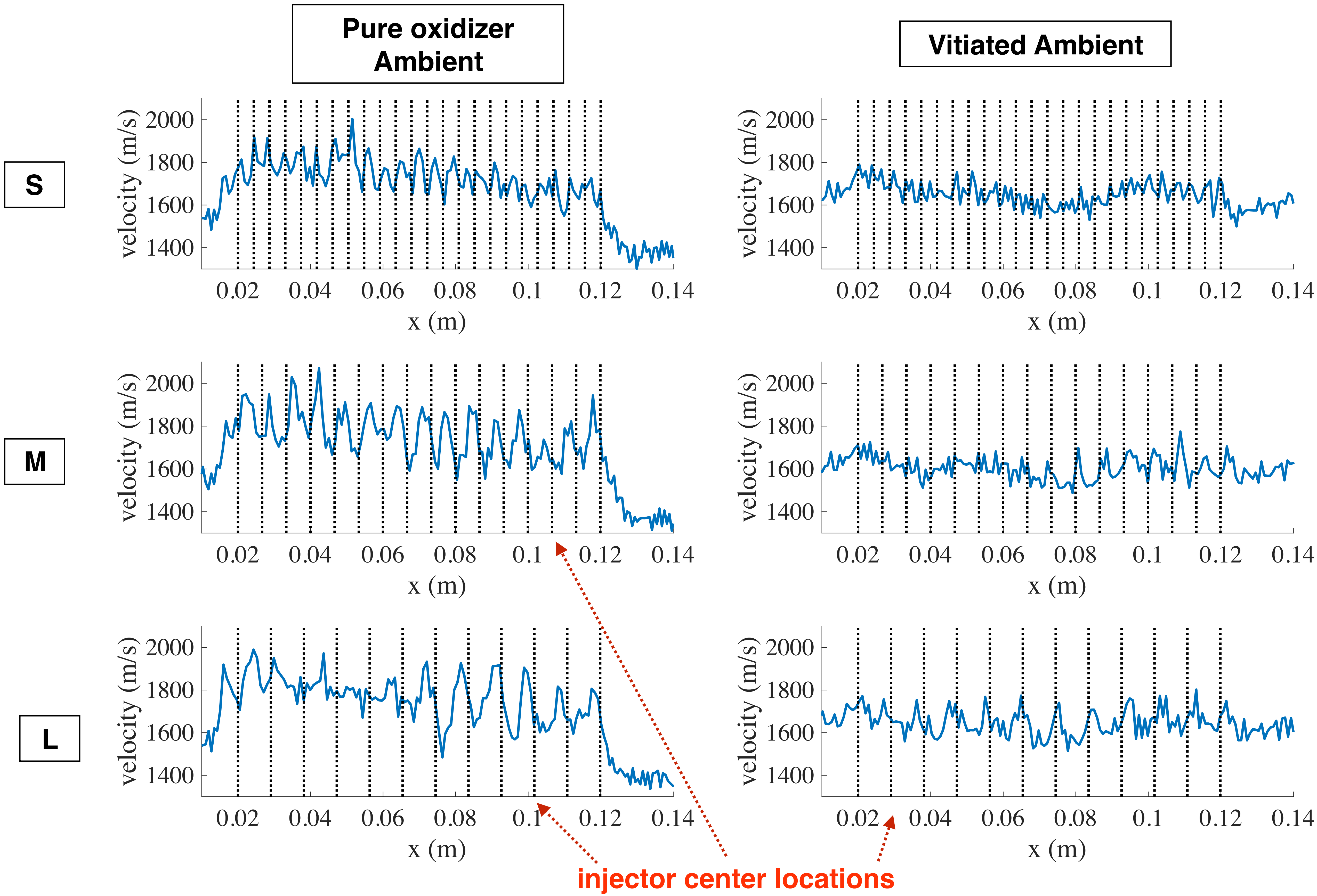
CONCENTRATION ALONG NORMAL



DISTANCE FROM FRONT (M)

- **Pressure jump used to identify detonation location**
  - ➡ Normal constructed from surface data
- **Mass fraction data extracted along the normal**

Detonation Velocity Variation



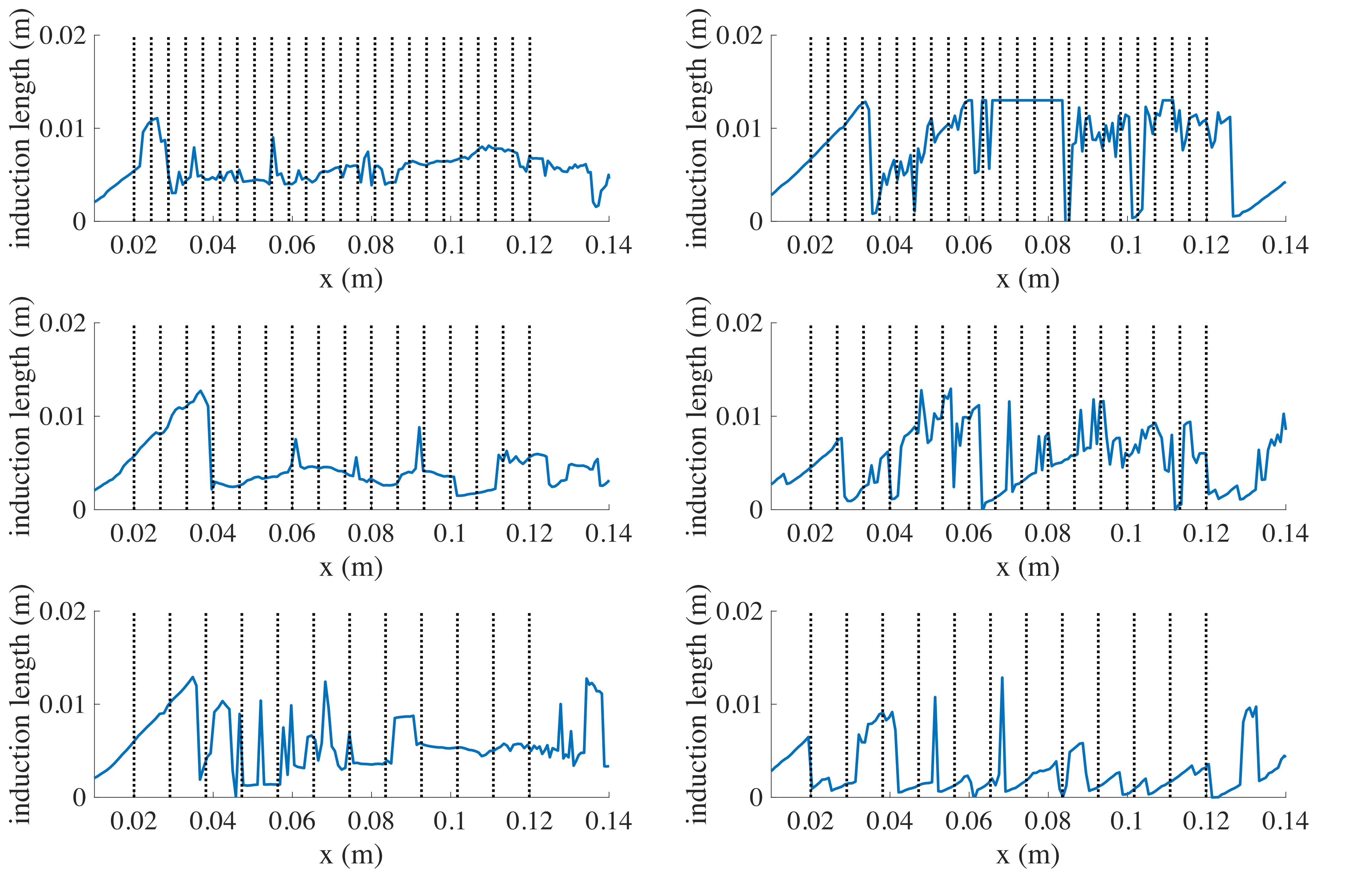
Induction Length

Pure oxidizer Ambient | **Vitiated Ambient**

S

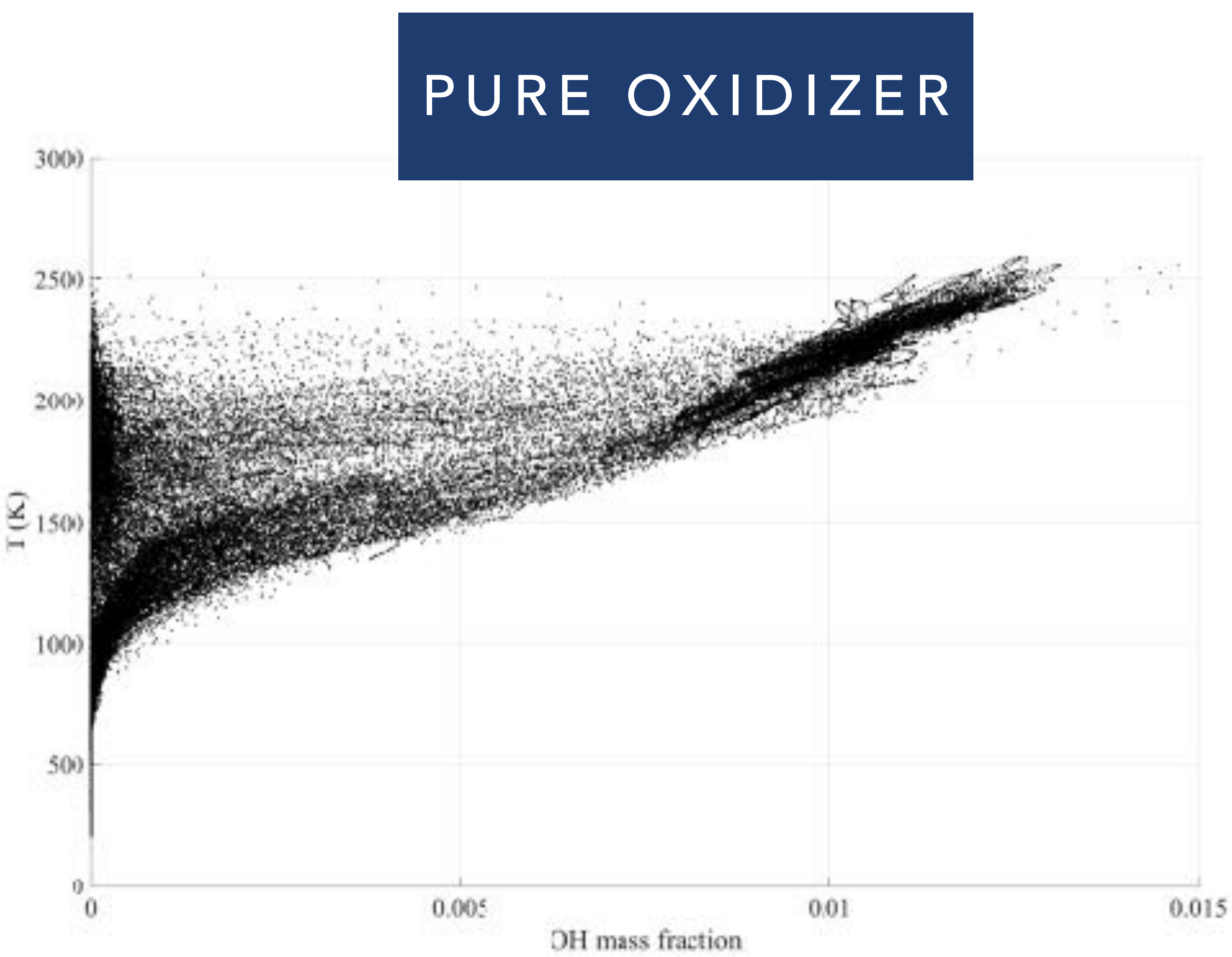
M

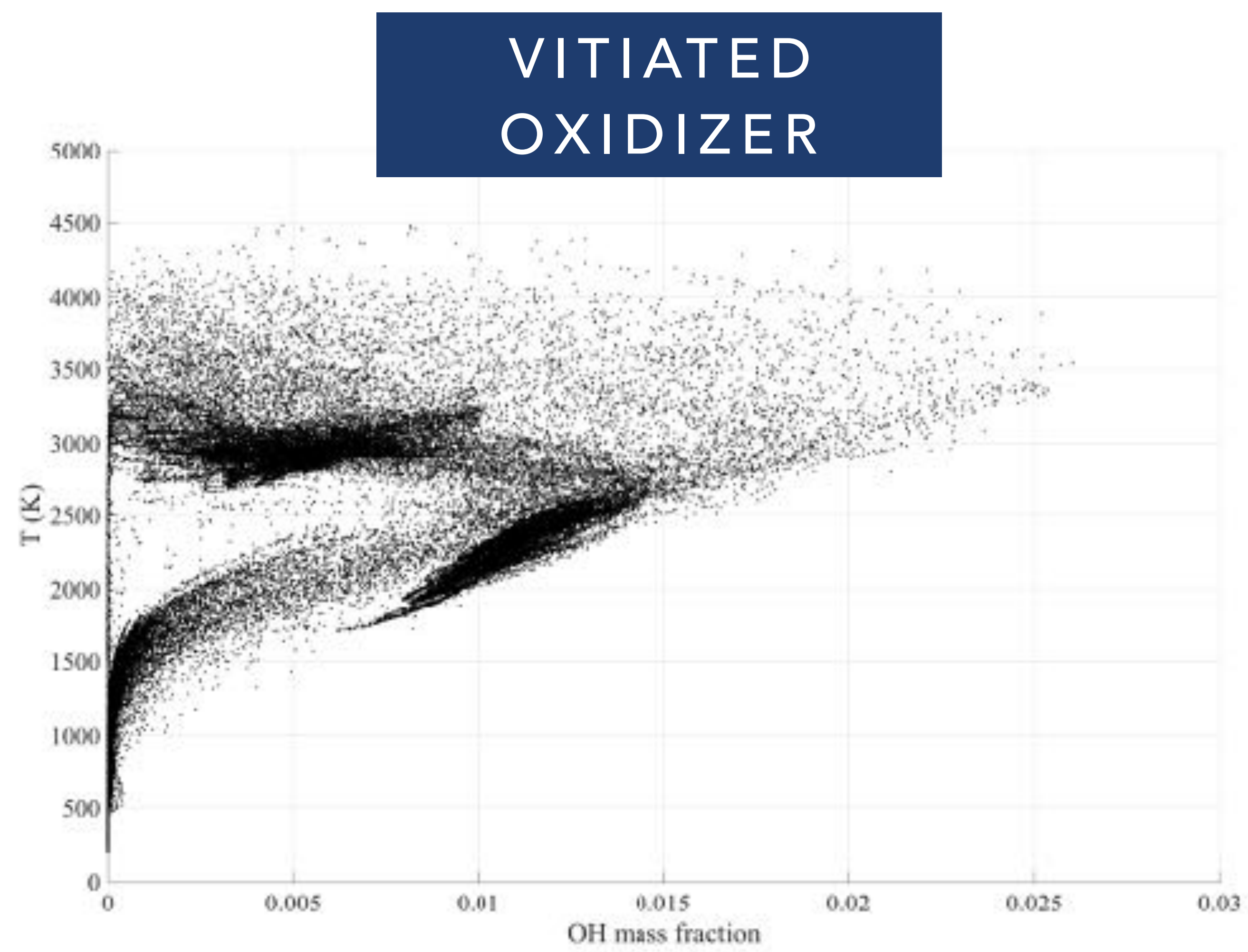
L



Conditional Scalar Plots

- **Conditional plots are useful in determining flame structure**
  - ➡ Obtained on the normal vector





Outlook for Year 2 & 3

- **Current progress**
  - ➡ Basic physics studies are close to completion
  - ➡ Next step is to extract combustion models based on DNS data
- **Year 2 - Full scale simulations**
  - ➡ Move to complex geometries and full-scale RDE simulations
  - ➡ OpenFOAM with AMR chosen as solver base
- **Year 3 - Optimization using inverse design**
  - ➡ Inverse design solver is being constructed